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* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAplus and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 12:53:52 ON 15 APR 2008

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:54:11 ON 15 APR 2008
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 14 APR 2008 HIGHEST RN 1014671-54-5
DICTIONARY FILE UPDATES: 14 APR 2008 HIGHEST RN 1014671-54-5

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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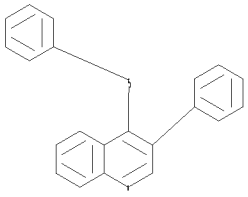
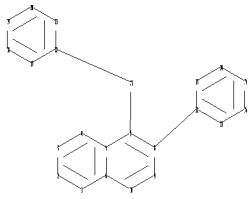
Uploading C:\Program Files\Stnexp\Queries\10-598,246.str





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23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
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7-23 8-12 22-23
ring bonds :
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14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
exact/norm bonds :
7-23 22-23
exact bonds :
8-12
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
containing 1 : 11 : 17 :

G1:O,S

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS

L1 STRUCTURE UPLOADED

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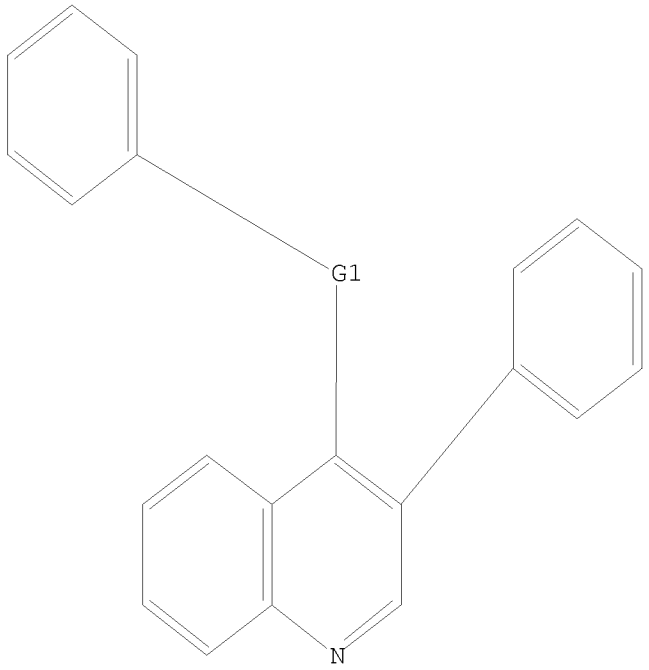
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1 sss sam
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SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9 TO 360
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

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=> s l1 sss full
FULL SEARCH INITIATED 12:55:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      122 TO ITERATE

100.0% PROCESSED      122 ITERATIONS                                25 ANSWERS
SEARCH TIME: 00.00.01

L3           25 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                     179.28     179.49

FILE 'CAPLUS' ENTERED AT 12:55:41 ON 15 APR 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)
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FILE COVERS 1907 - 15 Apr 2008  VOL 148 ISS 16
FILE LAST UPDATED: 14 Apr 2008  (20080414/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply.
They are available for your review at:

http://www.cas.org/infopolicy.html

=> s l3
L4           5 L3

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y
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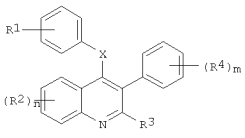
L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:979616 CAPLUS
DOCUMENT NUMBER: 143:266830
TITLE: Preparation of substituted quinoline compounds for use
as selective estrogen receptor modulator
INVENTOR(S): Hoekstra, William Joel; Miller, Aaron Bayne; Zuercher,
William John; Patel, Harikrishna Suryakant
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082857	A1	20050909	WO 2005-US5467	20050222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1727802	A1	20061206	EP 2005-723418	20050222
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV				
JP 2007523952	T	20070823	JP 2007-500908	20050222
US 20070203180	A1	20070830	US 2006-598246	20060822

PRIORITY APPLN. INFO.: US 2004-547544P P 20040225
WO 2005-US5467 W 20050222

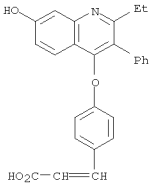
OTHER SOURCE(S): CASREACT 143:266830; MARPAT 143:266830
GI



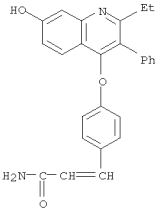
I

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

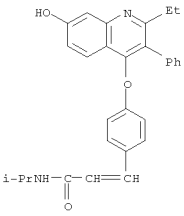
AB The present invention relates to novel compds. of Formula (I, variables defined below) with a variety of therapeutic uses, more particularly novel substituted quinoline compds. particularly useful for selective estrogen receptor modulation. For I, the variables are: R1 = CH=CH-R5; R5 = CN, C(O)OH, C(O)-N(R6)(R7); R6 and R7 = H, alkyl, aryl; or R6 and R7 may combine with the N to which they are attached to form a 3 to 7 membered optionally substituted ring; each R2 independently = H, halogen, haloalkyl, hydroxy, alkoxy, aryloxy, aralkyloxy, alkoxycarbonyloxy, aryloxycarbonyloxy, aralkyloxycarbonyloxy, alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or acyloxy; n = 1 or 2; R3 = H, OH, alkyl, alkoxy, aryloxy, aralkyloxy, haloalkylsulfonyloxy, halogen, haloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; X = O, S, S(O), or S(O)2; each R4 independently = H, halogen, haloalkyl, OH, alkoxy, aryloxy, aralkyloxy, alkoxycarbonyloxy, aryloxycarbonyloxy, aralkyloxycarbonyloxy, alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or acyloxy; and m = 1 or 2.
IT 828300-07-8P 828300-08-9P 828300-09-0P
828300-10-3P 828300-11-4P 828300-12-5P
828300-13-6P 828300-14-7P 863711-16-4P
863711-17-5P 863711-18-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of substituted quinoline compds. for use as selective estrogen receptor modulator to treat various diseases)
RN 828300-07-8 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



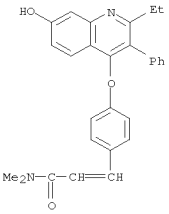
RN 828300-08-9 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



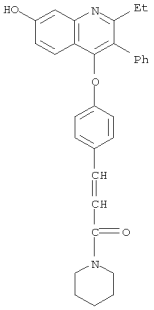
RN 828300-09-0 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- N-(1-methylethyl)- (CA INDEX NAME)



RN 828300-10-3 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- N,N-dimethyl- (CA INDEX NAME)

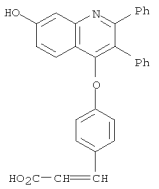


RN 828300-11-4 CAPLUS
CN Piperidine, 1-[3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)



RN 828300-12-5 CAPLUS
CN 2-Propenoic acid, 3-[4-[(7-hydroxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-13-6 CAPLUS
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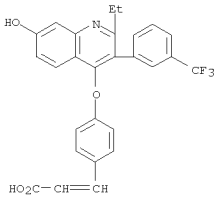
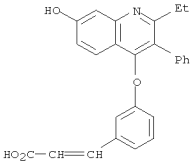


RN 828300-14-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 863711-16-4 CAPLUS
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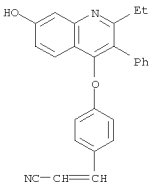
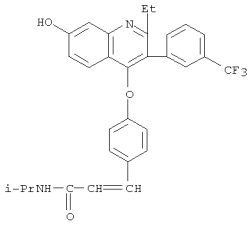


RN 863711-17-5 CAPLUS
CN 2-Propenamide, 3-[4-[[2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl]oxy]phenyl]-N-(1-methylethyl)- (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 863711-18-6 CAPLUS
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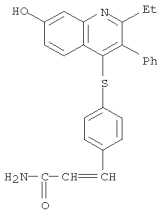
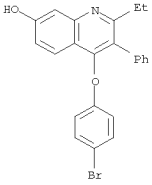
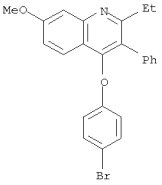


IT 863711-19-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted quinoline compds. for use as selective estrogen
receptor modulator to treat various diseases)
RN 863711-19-7 CAPLUS
CN 7-Quinolinol, 4-(4-bromophenoxy)-2-ethyl-3-phenyl- (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

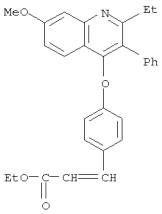


IT 828300-18-1P, 2-Ethyl-3-phenyl-4-(4-bromophenyloxy)-7-methoxyquinoline 828300-22-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted quinoline compds. for use as selective estrogen
receptor modulator to treat various diseases)
RN 828300-18-1 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



RN 828300-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2004:1070707 CAPLUS
DOCUMENT NUMBER: 142:212080
TITLE: Discovery of Novel Quinoline-Based Estrogen Receptor Ligands Using Peptide Interaction Profiling
AUTHOR(S): Hoekstra, William J.; Patel, Hari S.; Liang, Xi; Blanc, Jean-Baptiste E.; Heyer, Dennis O.; Willson, Timothy M.; Iannone, Marie A.; Kadwell, Sue H.; Miller, Lisa A.; Pearce, Kenneth H.; Simmons, Catherine A.; Shearin, Jean
CORPORATE SOURCE: GlaxoSmithKline Research Development, Research Triangle Park, NC, 27709-3398, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(6), 2243-2247
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:212080

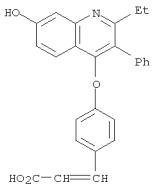
AB Traditional approaches to discovery of selective estrogen receptor modulators (SERMs) have relied on ER binding and cell-based estrogen response element-driven assays to identify compds. that are osteoprotective but nonproliferative in breast and uterine tissues. To discover new classes of potential SERMs, we have employed a cell-free microsphere-based binding assay to rapidly characterize ERα interactions with conformation-sensing cofactor or phage display peptides.

Peptide profiles of constrained triarenes were compared to known proliferative and nonproliferative ER ligands to discover potent quinoline-based ligands with minimal Ishikawa cell stimulation.

IT 828300-07-8P 828300-08-9P 828300-09-0P
828300-10-3P 828300-11-4P 828300-12-5P
828300-13-6P 828300-14-7P 828300-15-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)

RN 828300-07-8 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-08-9 CAPLUS
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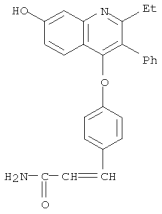

RN 828300-09-0 CAPLUS
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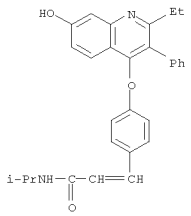
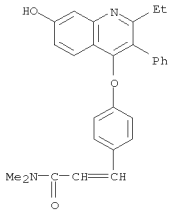
L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

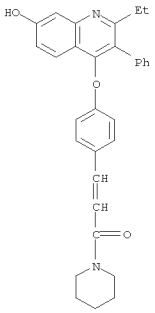


RN 828300-10-3 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N,N-dimethyl- (CA INDEX NAME)

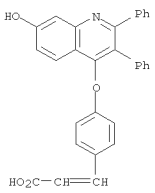


RN 828300-11-4 CAPLUS
CN Piperidine, 1-[3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

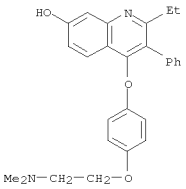


RN 828300-12-5 CAPLUS
CN 2-Propenoic acid,
3-[4-[(7-hydroxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]-
(CA INDEX NAME)

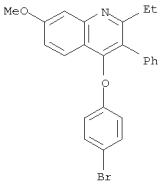


RN 828300-13-6 CAPLUS
CN 2-Propenoic acid,
3-[4-[[2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-
quinolinyl]oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

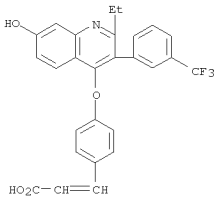


IT 828300-18-1P 828300-19-2P 828300-20-5P
828300-21-6P 828300-22-7P 828300-23-8P
828300-24-9P 828300-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)
(discovery of novel quinoline-based estrogen receptor ligands using
peptide interaction profiling)
RN 828300-18-1 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX
NAME)

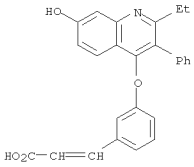


RN 828300-19-2 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-7-methoxy-2,3-diphenyl- (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

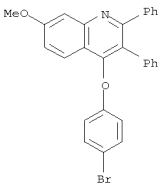


RN 828300-14-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-
quinolinyl)oxy]phenyl]- (CA INDEX NAME)

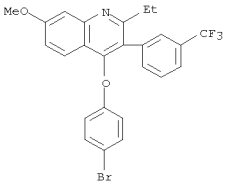


RN 828300-15-8 CAPLUS
CN 7-Quinolinol, 4-[4-[2-(dimethylamino)ethoxy]phenoxy]-2-ethyl-3-phenyl-
(CA INDEX NAME)

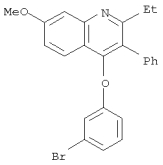
L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-20-5 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-[3-
(trifluoromethyl)phenyl]- (CA INDEX NAME)

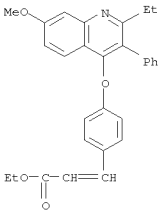


RN 828300-21-6 CAPLUS
CN Quinoline, 4-(3-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX
NAME)

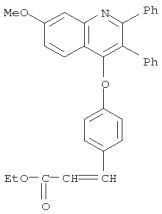


RN 828300-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-
quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

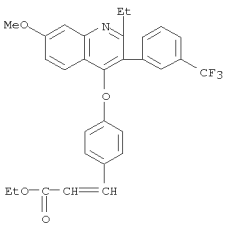


RN 828300-23-8 CAPLUS
CN 2-Propenoic acid,
3-[4-[(7-methoxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]-,
ethyl ester (CA INDEX NAME)

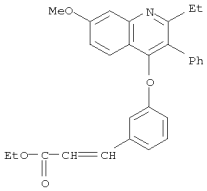


RN 828300-24-9 CAPLUS
CN 2-Propenoic acid,
3-[4-[[2-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]-4-
quinolinyl]oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-25-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-methoxy-3-phenyl-4-
quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

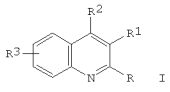


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

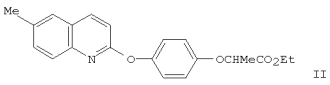
L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:598123 CAPLUS
DOCUMENT NUMBER: 97:198123
ORIGINAL REFERENCE NO.: 97:33181a,33184a
TITLE: Quinolineoxyphenoxypropionic acid derivatives and their use as herbicides
INVENTOR(S): Mildenberger, Hilmar; Knorr, Harald; Bauer, Klaus
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3101544	A1	19820819	DE 1981-3101544	19810120
PRIORITY APPLN. INFO.:			DE 1981-3101544	19810120

OTHER SOURCE(S): CASREACT 97:198123
GI



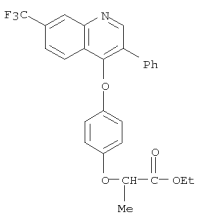
I



II

AB I [one of R or R2, especially R = 4-R4CHMeOC6H4O(R4 = CO2H or a derivative, e.g.
amide) and the other = H, C1-4 alkyl, Ph, Cl, Br; R1 = H, C1-4 alkyl, Cl, Br, cyano, C1-4 carbalkoxy; R3 = H, C1-4 alkyl alkoxy, or dialkylamino, NO2, CF3, halo; n = 0-2] were prepared as herbicides. Thus, 21 g 4-HOC6H4OCHMeCO2Et were added dropwise to 2.9 g NaH in 100 mL DMF, 17.7 g 2-chloro-6-methylquinoline added, and the mixture was stirred 2 h at 100° to give 89.2% II.
IT 83596-68-3P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 83596-68-3 CAPLUS
CN Propanoic acid, 2-[4-[[3-phenyl-7-(trifluoromethyl)-4-quinolinyl]oxy]phenoxy]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1956:24187 CAPLUS
DOCUMENT NUMBER: 50:24187
ORIGINAL REFERENCE NO.: 50:4954g-i,4955a-e
TITLE: A new method for the synthesis of certain benz[a]acridines
AUTHOR(S): Hauser, Charles R.; Murray, James G.
CORPORATE SOURCE: Duke Univ., Durham, NC
SOURCE: Journal of the American Chemical Society (1955), 77, 3858-60
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:24187

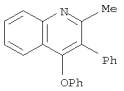
AB Certain 5-substituted benz[a]acridines were synthesized by acylating the Me group of 3-phenylquinaldine (I) or a derivative with an ester, and cyclizing the resulting ketone with polyphosphoric acid (II). PhCH2Ac (0.15 mol) and isatin were converted in the presence of alkali by the method of Borsche and Vorbach (C.A. 33, 1734.3) to 2-methyl-3-phenylcinchoninic acid, m. 338° (decomposition); the acid (50 g.) and 17 g. Cu powder, heated 2 h. at 340-50°, the mixture cooled, stirred with C6H6, and filtered, the solvent evaporated, and the residue distilled gave 35.4 g. I, yellow oil, b1.7 164°. I and (CO2Et)2 treated in the presence of KOEt by the method of Borsche and Vorbach (loc. cit.) gave Et (3-phenyl-2-quinolyl)pyruvate (III), orange needles, m. 161-3° (decomposition) (from EtOH). II (1.0 g.) and 10 g. II heated 15 min. at 195°, cooled to 85°, stirred with 20 cc. H2O, and filtered, the solid filter residue suspended in H2O, the mixture neutralized with 20% aqueous NaOH and filtered, and the residue triturated with hot 95% EtOH gave 0.67 g. benz[a]acridine-5-carboxylic acid (IV), yellow powder, m. 340° (decomposition); a 200-mg. portion sublimed gave 0.165 g. pure IV, m. 348° (decomposition). IV (0.100 g.) heated 0.5 h. with 0.1 g. Cu powder at 340° and the mixture sublimed at 140° and 0.5 mm. gave 0.047 g. benz[a]acridine (V), yellow needles, m. 132-3°. III (16.4 g.) in Et2O added to NaNH2 from 3.45 g. Na in liquid NH3, the mixture stirred 10 min., treated with 9.6 g. BzOMe in Et2O, stirred 4 h. at room temperature to evaporate the NH3, refluxed 0.5 h., diluted with H2O, and filtered, the Et2O layer of the filtrate evaporated to give addnl. solid, and the combined solids recrystd. from EtOH gave 12.0 g. 2-BzCH2 derivative (VI) of I, bright orange needles, m. 169-70° (from EtOH). VI (1 g.) heated 1.5 h. with 20 g. II at 195°, the mixture decomposed with H2O, neutralized with 20% aqueous NaOH, and extracted with Et2O, the extract washed, dried, and evaporated, and the residue recrystd. from 95% EtOH and dried on the steam bath yielded 0.82 g. 5-Ph derivative of V, yellow needles, m. 146-7° (sublimed at 160°/0.44 mm., recrystd. from 95% EtOH, and dried at 100°); picrate, yellow needles, m. 289-90° (from EtOH)

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

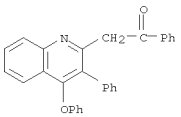
(decompn.). 4-Cl deriv. of I (20 g.), 9.3 g. PhONa, and 40 g. PhOH refluxed 4 h., the mixt. basified strongly with 20% aq. NaOH and extd. with Et2O, the ext. evapd., and the residue washed with 20% aq. NaOH and H2O and recrystd. from 95% EtOH gave 19.8 g. 4-PhO deriv. (VII) of I, colorless crystals, m. 123-6° (from 95% EtOH). VII (9.36 g.) in Et2O added to NaNH2 from 1.38 g. Na in liq. NH3, the mixt. stirred 5 min., treated with 8.16 g. BzOMe in Et2O, and stirred 1.5 h., the NH3 evapd., the residual Et2O suspension refluxed 8 h., dild. with H2O, and filtered, and the solid recrystd. from EtOH yielded 6.4 g. 4-PhO deriv. (VIII) of VI, orange plates, m. 185.5-87° (from EtOH). VIII (3 g.) heated 2.5 h. at 195° with 30 g. II, the mixt. decompd. with H2O and filtered, the residue suspended in 120 cc. N NaOH and extd. with Et2O, the ext. evapd., and the residue recrystd. from 95% EtOH yielded 1.60 g. 5-phenyl-12-phenoxy deriv. (IX) of V, light yellow crystals, m. 207-9°. IX hydrolyzed with HBr gave 12(7H)-oxo deriv. (X) of 5-phenylbenz[a]acridine (XI). The crude solid (1.0 g.) from VIII and II refluxed with 5 cc. 48% HBr, 20 cc. EtOH, and 5 cc. H2O 3 h. with stirring, the mixt. neutralized with NaOH and filtered, and the solid washed with H2O and Et2O and triturated with hot EtOH gave 0.39 g. X, m. 342° (decompn.) (sublimed). X (0.25 g.) heated with 20 g. Zn dust to red heat and the distillate (collected on the wall of the combustion tube) sublimed at 160° and 0.4 mm. and recrystd. from EtOH gave XI, m. 146-6.5°.

IT 5350-65-2P, Quinaldine, 4-phenoxy-3-phenyl- 652972-11-7P , Acetophenone, 2-(4-phenoxy-3-phenyl-2-quinolyl)-
RL: PREP (Preparation)
(preparation of)

RN 5350-65-2 CAPLUS
CN Quinoline, 2-methyl-4-phenoxy-3-phenyl- (CA INDEX NAME)



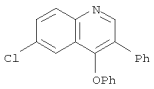
RN 652972-11-7 CAPLUS
CN Acetophenone, 2-(4-phenoxy-3-phenyl-2-quinolyl)- (5CI) (CA INDEX NAME)



L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1951:36166 CAPLUS
DOCUMENT NUMBER: 45:36166
ORIGINAL REFERENCE NO.: 45:6204f-i,6205a-b
TITLE: Some 4-(dialkylaminoalkylamino)-3-phenylquinolines
AUTHOR(S): Adams, W. J.; Hey, D. H.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society (1950) 3254-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB The amine (1 mol.) is added to 1 mol. HCOCHPhCO2Et (I) at room temperature (slight warming in the case of solid amines), kept 24 hrs. at room temperature, the product extracted with ether, and the oil added to boiling Ph2O and heated for varying times, giving 21-55% of the following 4-hydroxy-3-phenylquinolines (II): 6-Cl, m. 349-9.5° (decomposition); 8-Cl, cream, m. 248-51°; 6-Br, cream, m. 365° (decomposition); 6-NO2, yellow, m. 349-50° (decomposition); 8-NO2, bright orange, m. 215-16°; 6-MeO, m. 337-8° (decomposition). The II (1 mol.) and 1 mol. PCl5 in POCl3 were heated from 25 min. to 1.5 hrs., giving the 4-chloro-3-phenylquinolines (III): 6-Cl, m. 144.5°; 8-Cl, m. 112.5-13.5°; 6-NO2, pale brown, m. 170.5-2°; 6-MeO, yellow, m. 138-8.5° (picrate, yellow, m. 206-7°); in 1 experiment the product was 4,x-dichloro-6-methoxy-3-phenylquinoline, m. 131-1.5°. 4-Chloro-3-phenylquinoline (0.5 g.) and 0.2 g. PhNH2, heated 5 min. at 130° and the product extracted with 5% HCl, give the HCl salt, bright yellow, m. 300°, of 4-anilino-3-phenylquinoline (IV), cream, m. 179.5-80.5°; 6-MeO derivative, cream, m. 172-3°. The III (1 mol.) and 2.5 mols. of the amine were heated 4 hrs. at 160-80° and 4 hrs. at 210°, the excess amine removed in vacuo, the residue extracted with 66% aqueous AcOH, the solution made alkaline with 10% aqueous NaOH, the oil extracted with ether, diluted with AcOH, and the base precipitated with picric acid, giving the dipicrates of 3-phenylquinolines (the Me2CO of crystallization is removed at 100° in vacuo but not at 80° at atmospheric pressure): 4-(2-diethylaminoethylamino), m. 201.5-2.5° (all m. with decomposition) (6-Cl derivative, with 1 mol. Me2CO, m. 202.5-4.5°; 7-Cl derivative, with 1 mol. Me2CO, m. 205-6°; 6-MeO derivative, with 1 mol. Me2CO, m. 170-3°); 4-(4-diethylamino-1-methylbutylamino), m. 213-15°; 6-Cl derivative with 1 mol. Me2CO, m. 210-18°; 7-Cl derivative, with 1 mol. Me2CO, m. 205-6°; 6-MeO derivative, with 1 mol. Me2CO, m. 194-5°. 6-Chloro-4-phenoxy-3-phenylquinoline, m. 152.5-3.5°. α-Phenyl-p-acetanisidide m. 122-3° (from PhCH2COCl and p-MeOC6H4NH2). Impure I and amines give α-phenylacetanilides. PhNH2 (1.9 g.) and 3.8 g. I, 24 hrs. at room temperature, give 48% 4-hydroxy-3-phenylquinoline (V), and 0.7 g. IV; the reactants, 30 min. at room temperature and 24 hrs. at room temperature, give 45% V and 0.5 g. IV; heating 30 min. at 100° and keeping 24 hrs. at room temperature gives 34% V and 0.2 g. IV; thus, temperature has little effect on the reaction. I and PhNH2 (0.02 mol. each) give 41% V; 0.02 mol. I and 0.018

L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
mol. PhNH2 give 59% V; 0.02 mol. I and 0.04 mol. PhNH2 give 5% V, 22% IV, and 1.7 g. (PhNH)2CO. The PhNHCH:CPhCO2Et (from 3.8 g. I and 1.7 g. PhNH2), cyclized in 20 or 40 cc. Ph2O, gives 47 and 81% V, resp.
IT 860719-92-2P, Quinoline, 6-chloro-4-phenoxy-3-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 860719-92-2 CAPLUS
CN Quinoline, 6-chloro-4-phenoxy-3-phenyl- (CA INDEX NAME)



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NEWS 5	JAN 28	MARPAT searching enhanced
NEWS 6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
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NEWS 12	FEB 25	IMSPRODUCT reloaded with enhancements

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 NEWS IPC8     For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that
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FILE 'HOME' ENTERED AT 14:51:10 ON 16 APR 2008

=> FIL REGISTRY
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                         ENTRY    SESSION
FULL ESTIMATED COST                                       0.21       0.21

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.
```

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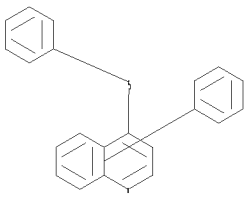
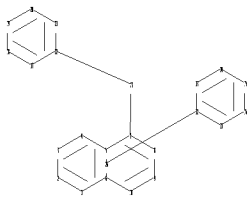
http://www.cas.org/support/stngen/stndoc/properties.html

=>
Uploading C:\Program Files\Stnexp\Queries\10-598,246a.str





chain nodes :
23
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22
chain bonds :
7-23 22-23
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22

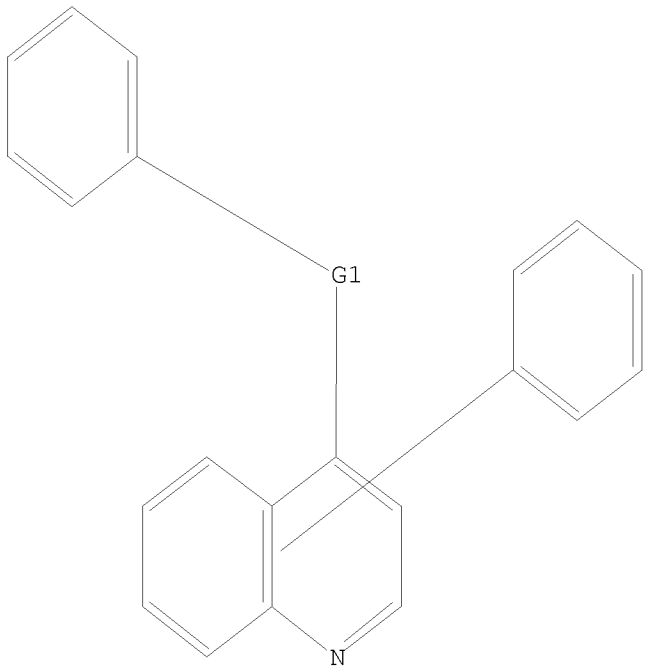
exact/norm bonds :
7-23 22-23
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 11-12 11-16 12-13 13-14
14-15 15-16 17-18 17-22 18-19 19-20 20-21 21-22
isolated ring systems :
containing 1 : 11 : 17 :

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 21:Atom 22:Atom 23:CLASS 26:Atom

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

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=> s l1 sss sam
SAMPLE SEARCH INITIATED 14:52:24 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      469 TO ITERATE

100.0% PROCESSED      469 ITERATIONS                                3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         8081 TO    10679
PROJECTED ANSWERS:               3 TO      163

L2            3 SEA SSS SAM L1

=> s l1 sss full
FULL SEARCH INITIATED 14:52:36 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -     9410 TO ITERATE

100.0% PROCESSED     9410 ITERATIONS                            105 ANSWERS
SEARCH TIME: 00.00.01

L3          105 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                     ENTRY    SESSION
FULL ESTIMATED COST                                178.82     179.03

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=> s l3
```

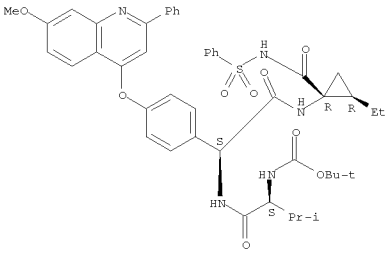
L4 25 L3

=> d ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 25 ANSWERS - CONTINUE? Y/(N):y

L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:1398918 CAPLUS
DOCUMENT NUMBER: 148:138206
TITLE: Effects on protease inhibition by modifying of helicase residues in hepatitis C virus nonstructural protein 3
AUTHOR(S): Dahl, Goeran; Sandstroem, Anja; Aakerblom, Eva; Danielson, U. Helena
CORPORATE SOURCE: Department of Biochemistry and Organic Chemistry, Uppsala University, Swed.
SOURCE: FEBS Journal (2007), 274(22), 5979-5986
CODEN: FJEOAC; ISSN: 1742-464X
PUBLISHER: Blackwell Publishing Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This study of the full-length bifunctional nonstructural protein 3 from hepatitis C virus (HCV) has revealed that residues in the helicase domain affect the inhibition of the protease. Two residues (Q526 and H528), apparently located in the interface between the S2 and S4 binding pockets of the substrate binding site of the protease, were selected for modification, and three enzyme variants (Q526A, H528A and H528S) were expressed, purified and characterized. The substitutions resulted in indistinguishable Km values and slightly lower kcat values compared to the wild-type. The Ki values for a series of structurally diverse protease inhibitors were affected by the substitutions, with increases or decreases up to 10-fold. The inhibition profiles for H528A and H528S were different, confirming that not only did the removal of the imidazole side chain have an effect, but also that minor differences in the nature of the introduced side chain influenced the characteristics of the enzyme. These results indicate that residues in the helicase domain of nonstructural protein 3 can influence the protease, supporting our hypothesis that full-length hepatitis C virus nonstructural protein 3 should be used for protease inhibitor optimization and characterization. Furthermore, the data suggest that inhibitors can be designed to interact with residues in the helicase domain, potentially leading to more potent and selective compds.
IT 1001331-39-0
RL: ARU (Analytical role, unclassified); BSU (Biological study, unclassified); ANST (Analytical study); BIOL (Biological study)
(inhibitor NS3 protease activity; identification of residues in helicase domain of HCV protein NS3 that affect inhibition of protease activity)
RN 1001331-39-0 CAPLUS
CN Carbamic acid, N-[(1S)-1-[[[(1S)-2-[[(1R,2R)-2-ethyl-1-[[(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-2-oxoethyl]amino]carbonyl]-2-methylpropyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.

L4 ANSWER 1 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

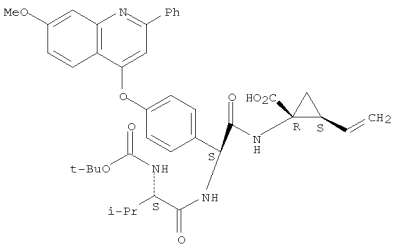


REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:24155 CAPLUS
DOCUMENT NUMBER: 146:287649
TITLE: Phenylglycine as a novel P2 scaffold in hepatitis C virus NS3 protease inhibitors
AUTHOR(S): Oertqvist, Pernilla; Peterson, Shane D.; Aakerblom, Eva; Gossas, Thomas; Sabnis, Yogesh A.; Fransson, Rebecca; Lindeberg, Gunnar; Danielson, U. Helena; Karlen, Anders; Sandstroem, Anja
CORPORATE SOURCE: Department of Medicinal Chemistry, BMC, Uppsala University, Uppsala, SE-751 23, Swed.
SOURCE: Bioorganic & Medicinal Chemistry (2007), 15(3), 1448-1474
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 146:287649
AB Mol. modeling and inhibitory potencies of tetrapeptide protease inhibitors of HCV NS3 proposed phenylglycine as a new promising P2 residue. The results suggest that phenylglycine might be capable of interacting with the NS3 (protease-helicase/NTPase) in ways not possible for the common P2 proline-based inhibitors. Thus, a series of tripeptides, both linear and macrocyclic, based on p-hydroxy-phenylglycine in the P2 position were prepared and their inhibitory effect determined When the p-hydroxy group was replaced by methoxy, isoquinolin-, or quinolinyloxy functions, inhibitors with improved potencies were obtained. The P2 phenylglycine-based inhibitors were further optimized by C-terminal extension to acyl sulfonamides and by P1-P3 cyclization, which gave products with inhibition consts. in the nanomolar range (.apprx.75 nM).
IT 928162-22-5P 928162-23-6P 928162-57-6P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(hepatitis C virus NS3 protease inhibitors preparation: phenylglycine as a novel P2 scaffold)
RN 928162-22-5 CAPLUS
CN Cyclopropanecarboxylic acid, N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-2-ethenyl-, (1R,2S)- (CA INDEX NAME)

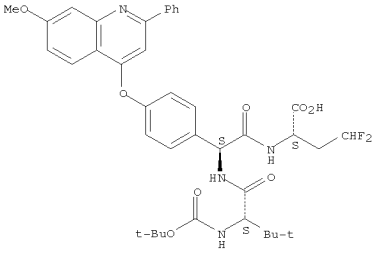
Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-23-6 CAPLUS
CN Butanoic acid, N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-2-amino-4,4-difluoro-, (2S)- (CA INDEX NAME)

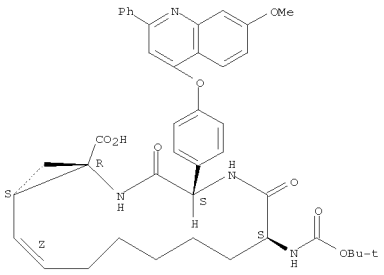
Absolute stereochemistry.



RN 928162-57-6 CAPLUS
CN 2,5-Diazabicyclo[13.1.0]hexadec-13-ene-1-carboxylic acid, 7-[[(1,1-dimethylethoxy)carbonyl]amino]-4-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-3,6-dioxo-, (1R,4S,7S,13Z,15S)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

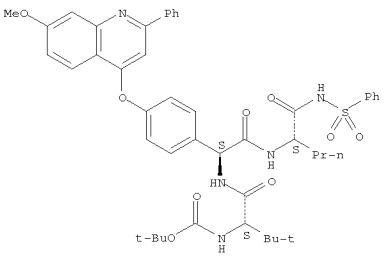
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



IT 928162-36-1P 928162-37-2P 928162-38-3P
928162-39-4P 928162-40-7P 928162-46-3P
928162-47-4P 928162-60-1P 928162-61-2P
928162-66-7P
RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(hepatitis C virus NS3 protease inhibitors preparation: phenylglycine as
novel P2 scaffold)
RN 928162-36-1 CAPLUS
CN L-Norvalinamide,
N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-
[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-N-(phenylsulfonyl)-
(CA INDEX NAME)

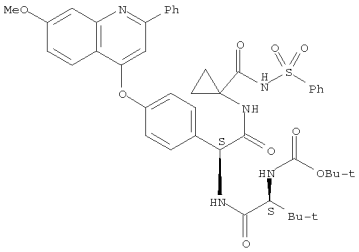
Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-37-2 CAPLUS
CN Cyclopropanecarboxamide,
N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-
(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-N-
(phenylsulfonyl)- (CA INDEX NAME)

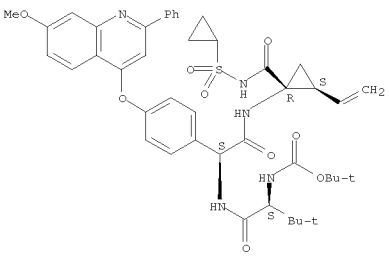
Absolute stereochemistry.



RN 928162-38-3 CAPLUS
CN Cyclopropanecarboxamide,
N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-
(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-N-
(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)

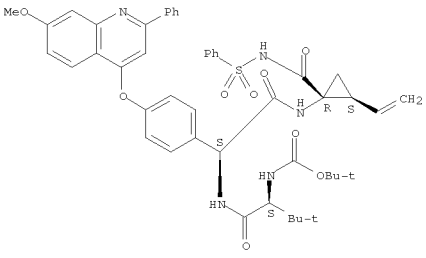
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

Absolute stereochemistry.



RN 928162-39-4 CAPLUS
CN Cyclopropanecarboxamide,
N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-
(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-2-
ethenyl-N-(phenylsulfonyl)-, (1R,2S)- (CA INDEX NAME)

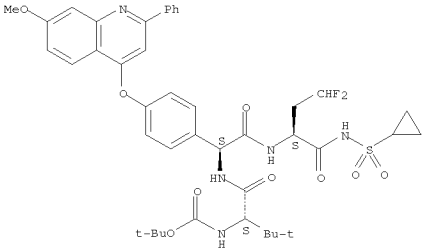
Absolute stereochemistry.



RN 928162-40-7 CAPLUS
CN Butanamide, N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-
[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-2-amino-N-
(cyclopropylsulfonyl)-4,4-difluoro-, (2S)- (CA INDEX NAME)

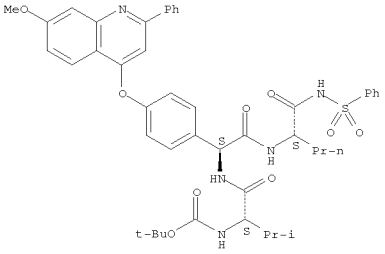
Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-46-3 CAPLUS
CN L-Norvalinamide, N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-N-(phenylsulfonyl)- (CA INDEX NAME)

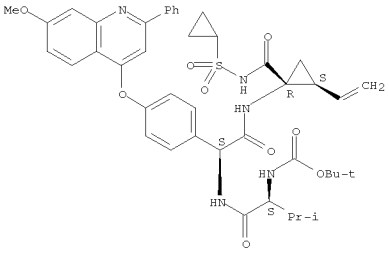
Absolute stereochemistry.



RN 928162-47-4 CAPLUS
CN Cyclopropanecarboxamide, N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-N-(cyclopropylsulfonyl)-2-ethenyl-, (1R,2S)- (CA INDEX NAME)

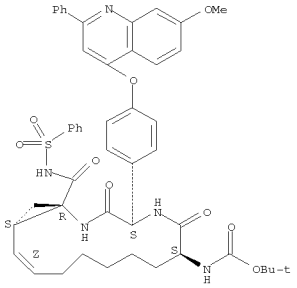
Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



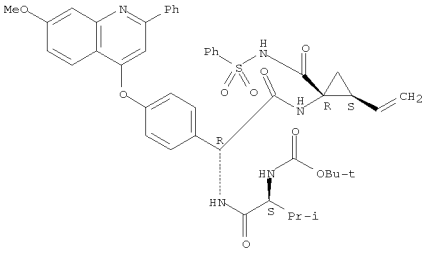
RN 928162-60-1 CAPLUS
CN Carbamic acid, N-[(1R,4S,7S,13Z,15S)-4-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-3,6-dioxo-1-[[(phenylsulfonyl)amino]carbonyl]-2,5-diazabicyclo[13.1.0]hexadec-13-en-7-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



RN 928162-61-2 CAPLUS
CN Carbamic acid,
N-[(1R,4S,7S,13Z,15S)-1-[[(cyclopropylsulfonyl)amino]carbon

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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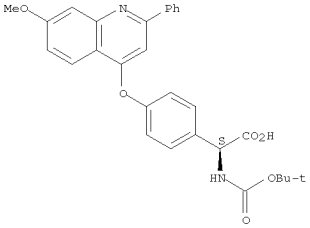
928162-26-9P 928162-27-0P 928162-28-1P
928162-29-2P 928162-51-0P 928162-54-3P
945904-18-7P 945904-35-8P 945904-95-0P
945905-14-6P 945905-16-8P 945905-32-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hepatitis C virus NS3 protease inhibitors preparation: phenylglycine as
novel P2 scaffold)
RN 928162-13-4 CAPLUS
CN Benzeneacetic acid, α-[[(1,1-dimethylethoxy)carbonyl]amino]-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-, (αS)- (CA INDEX NAME)

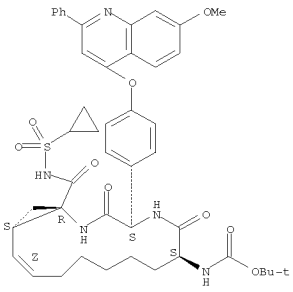
Absolute stereochemistry.



RN 928162-18-9 CAPLUS
CN Cyclopropanecarboxylic acid, 1-[[(2S)-2-[[(1,1-

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
yl]-4-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-3,6-dioxo-2,5-diazabicyclo[13.1.0]hexadec-13-en-7-yl]-, 1,1-dimethylethyl ester (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

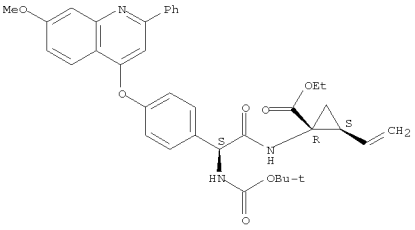


RN 928162-66-7 CAPLUS
CN Cyclopropanecarboxamide, N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2R)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-2-ethenyl-N-(phenylsulfonyl)-, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.

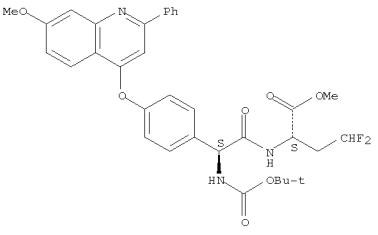
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
dimethylethoxy)carbonyl]amino]-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]acetyl]amino]-2-ethenyl-, ethyl ester, (1R,2S)-(CA
INDEX NAME)

Absolute stereochemistry.



RN 928162-19-0 CAPLUS
CN Butanoic acid, 2-[[(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]acetyl]amino]-4,4-difluoro-, methyl ester, (2S)- (CA INDEX NAME)

Absolute stereochemistry.

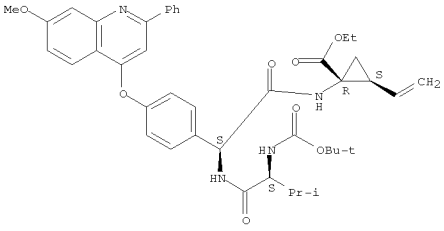


RN 928162-20-3 CAPLUS
CN Cyclopropanecarboxylic acid,
N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2S)-

2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-2-ethenyl-, ethyl ester, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.

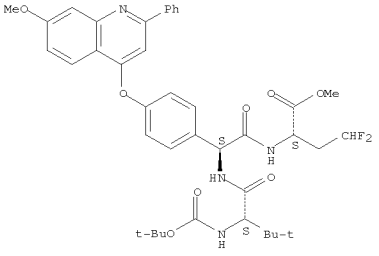
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-21-4 CAPLUS
CN Butanoic acid,
N-[(1,1-dimethylethoxy)carbonyl]-3-methyl-L-valyl-(2S)-2-[4-

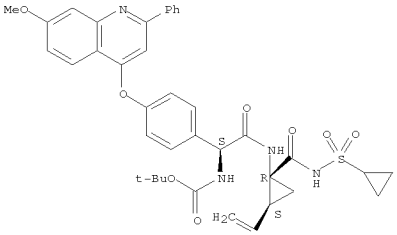
[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-2-amino-4,4-difluoro-,
methyl ester, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



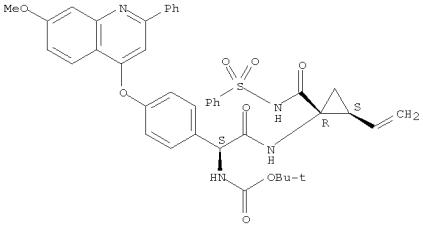
RN 928162-25-8 CAPLUS
CN Carbamic acid,
N-[(1S)-1-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-
2-oxo-2-[[(1S)-1-[[(phenylsulfonyl)amino]carbonyl]butyl]amino]ethyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-28-1 CAPLUS
CN Carbamic acid, N-[(1S)-2-[[(1R,2S)-2-ethenyl-1-
[[(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]-1-[4-[(7-methoxy-2-
phenyl-4-quinolinyl)oxy]phenyl]-2-oxoethyl]-, 1,1-dimethylethyl ester
(CA
INDEX NAME)

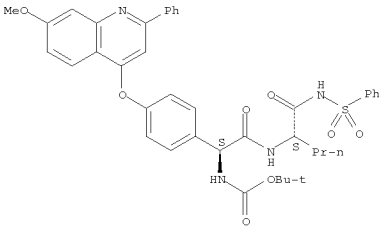
Absolute stereochemistry.



RN 928162-29-2 CAPLUS
CN Carbamic acid, N-[(1S)-2-[[(1S)-1-[[(cyclopropylsulfonyl)amino]carbonyl]-
3,3-difluoropropyl]amino]-1-[4-[(7-methoxy-2-phenyl-4-
quinolinyl)oxy]phenyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (CA INDEX
NAME)

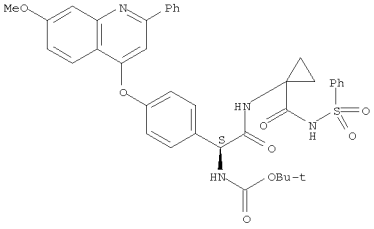
Absolute stereochemistry.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
Absolute stereochemistry.



RN 928162-26-9 CAPLUS
CN Carbamic acid,
N-[(1S)-1-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]-
2-oxo-2-[[1-[[(phenylsulfonyl)amino]carbonyl]cyclopropyl]amino]ethyl]-,
1,1-dimethylethyl ester (CA INDEX NAME)

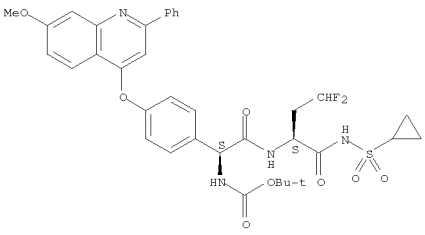
Absolute stereochemistry.



RN 928162-27-0 CAPLUS
CN Carbamic acid,
N-[(1S)-2-[[(1R,2S)-1-[[(cyclopropylsulfonyl)amino]carbonyl
]-2-ethenylcyclopropyl]amino]-1-[4-[(7-methoxy-2-phenyl-4-
quinolinyl)oxy]phenyl]-2-oxoethyl]-, 1,1-dimethylethyl ester (CA INDEX
NAME)

Absolute stereochemistry.

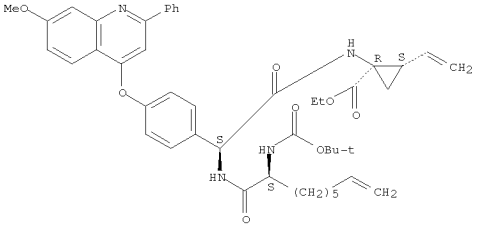
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 928162-51-0 CAPLUS
CN Cyclopropanecarboxylic acid, 1-[[(2S)-2-[[(2S)-2-[[(1,1-

dimethylethoxy)carbonyl]amino]-1-oxo-8-nonen-1-yl]amino]-2-[4-[(7-methoxy-
2-phenyl-4-quinolinyl)oxy]phenyl]acetyl]amino]-2-ethenyl-, ethyl ester,
(1R,2S)- (CA INDEX NAME)

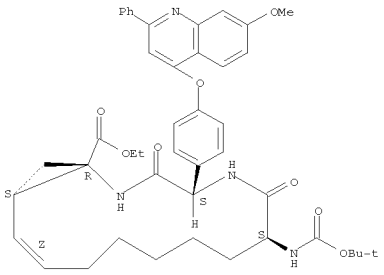
Absolute stereochemistry.



RN 928162-54-3 CAPLUS
CN 2,5-Diazabicyclo[13.1.0]hexadec-13-ene-1-carboxylic acid,
7-[[(1,1-dimethylethoxy)carbonyl]amino]-4-[4-[(7-methoxy-2-phenyl-4-
quinolinyl)oxy]phenyl]-3,6-dioxo-, ethyl ester, (1R,4S,7S,13Z,15S)- (CA
INDEX NAME)

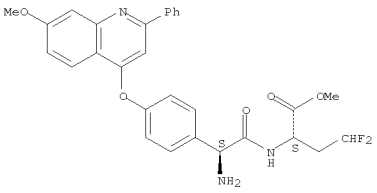
Absolute stereochemistry.
Double bond geometry as shown.

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 945904-18-7 CAPLUS
CN Butanoic acid, 2-[[(2S)-2-amino-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]acetyl]amino]-4,4-difluoro-, methyl ester, (2S)- (CA INDEX NAME)

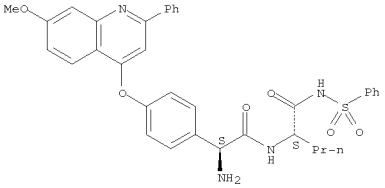
Absolute stereochemistry.



RN 945904-35-8 CAPLUS
CN Benzeneacetamide, α-amino-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-N-[(1S)-1-[[(phenylsulfonyl)amino]carbonyl]butyl]-, hydrochloride (1:1), (αS)- (CA INDEX NAME)

Absolute stereochemistry.

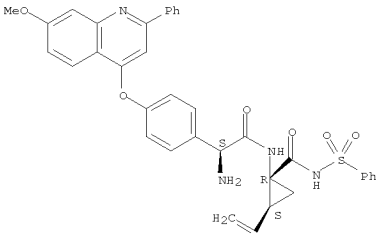
L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



● HCl

RN 945904-95-0 CAPLUS
CN Benzeneacetamide, α-amino-N-[(1R,2S)-2-ethenyl-1-[[(phenylsulfonyl)amino]carbonyl]cyclopropyl]-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-, hydrochloride (1:1), (αS)- (CA INDEX NAME)

Absolute stereochemistry.

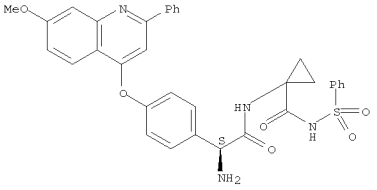


● HCl

RN 945905-14-6 CAPLUS
CN Benzeneacetamide, α-amino-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-N-[1-[[(phenylsulfonyl)amino]carbonyl]cyclopropyl]-, hydrochloride (1:1), (αS)- (CA INDEX NAME)

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

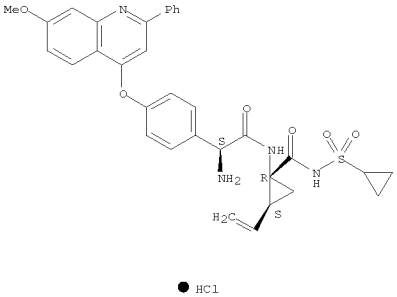
Absolute stereochemistry.



● HCl

RN 945905-16-8 CAPLUS
CN Benzeneacetamide, α-amino-N-[(1R,2S)-1-[[(cyclopropylsulfonyl)amino]carbonyl]-2-ethenylcyclopropyl]-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-, hydrochloride (1:1), (αS)- (CA INDEX NAME)

Absolute stereochemistry.

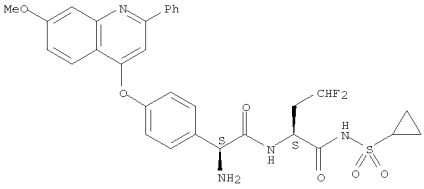


● HCl

RN 945905-32-8 CAPLUS
CN Benzeneacetamide, α-amino-N-[(1S)-1-[[(cyclopropylsulfonyl)amino]carbonyl]-3,3-difluoropropyl]-4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]-, hydrochloride (1:1), (αS)- (CA INDEX NAME)

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

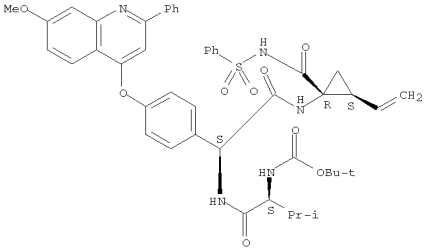
Absolute stereochemistry.



● HCl

IT 928162-65-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(hepatitis C virus NS3 protease inhibitors preparation: phenylglycine as
novel P2 scaffold)
RN 928162-65-6 CAPLUS
CN Cyclopropanecarboxamide, N-[(1,1-dimethylethoxy)carbonyl]-L-valyl-(2S)-2-[4-[(7-methoxy-2-phenyl-4-quinolinyl)oxy]phenyl]glycyl-1-amino-2-ethenyl-N-(phenylsulfonyl)-, (1R,2S)- (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 64 THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

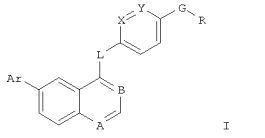
ACCESSION NUMBER: 2005:1329589 CAPLUS
DOCUMENT NUMBER: 144:69746
TITLE: Preparation of quinoline and isoquinoline-based compounds exhibiting ATP-utilizing enzyme inhibitory activity, and compositions, and uses thereof
INVENTOR(S): Dickson, John K., Jr.; Williams, Kevin P.; Hodge, Carl
Nicholas
PATENT ASSIGNEE(S): Amphora Discovery Corporation, USA
SOURCE: PCT Int. Appl., 106 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005120509	A1	20051222	WO 2005-US19255	20050603
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2005251735	A1	20051222	AU 2005-251735	20050603
CA 2569404	A1	20051222	CA 2005-2569404	20050603
US 20060009460	A1	20060112	US 2005-145562	20050603
EP 1781293	A1	20070509	EP 2005-755909	20050603
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2008501696	T	20080124	JP 2007-515534	20050603

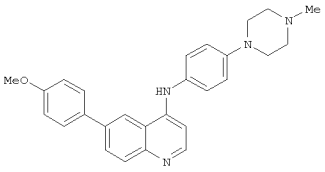
PRIORITY APPLN. INFO.: US 2004-577224P P 20040604
WO 2005-US19255 W 20050603

OTHER SOURCE(S): CASREACT 144:69746; MARPAT 144:69746
GI

L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



I



II

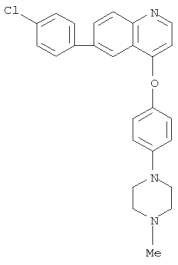
AB Preparation of title compds. I [Ar = (un)substituted hetero/aryl; A = N and B =
CH; or A = CH and B = N; L = O, NH and derivs.; X, Y = independently CH, N; G = a covalent bond, NH and derivs.; R = (un)substituted heterocycloalkyl; with the proviso that when Ar = Ph, A = N, B = CH, L = NH, X = Y = CH, and G = a covalent bond, then R is not 4-methylpiperazin-1-yl], and their pharmaceutically acceptable salts, solvates, chelates, non-covalent complexes, prodrugs, and mixts., exhibiting ATP-utilizing enzyme inhibitory activity (no data), methods of using them, and compns. containing them are described. For example, a 3-step
synthesis, from 1-fluoro-4-nitrobenzene and N-methylpiperazine, is given for quinoline II. I displayed selective activity for one of the following
protein kinases or pair of protein kinases: AKT1, CDK2/cyclin A, DAPK1, ABL1, etc. (no data). I are useful for the treatment of at least one of the diseases selected from Alzheimer's disease, stroke, diabetes, obesity,
inflammation, Crohn's disease, cancer, etc. (no data).

IT 871874-03-2P, 6-(4-Chlorophenyl)-4-[4-(4-methylpiperazin-1-yl)phenoxy]quinoline 871874-04-3P, 4-[4-[4-(4-Methylpiperazin-1-yl)phenoxy]quinolin-6-yl]benzonitrile
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of quinoline and isoquinoline-based compds.
exhibiting ATP-utilizing enzyme inhibitory activity and their compns. and uses)

RN 871874-03-2 CAPLUS

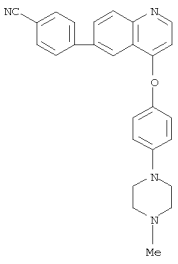
L4 ANSWER 3 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

CN Quinoline, 6-(4-chlorophenyl)-4-[4-(4-methyl-1-piperazinyl)phenoxy]- (CA INDEX NAME)



RN 871874-04-3 CAPLUS

CN Benzonitrile, 4-[4-[4-(4-methyl-1-piperazinyl)phenoxy]-6-quinolinyl]- (CA INDEX NAME)



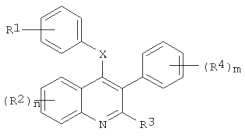
REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:979616 CAPLUS
DOCUMENT NUMBER: 143:266830
TITLE: Preparation of substituted quinoline compounds for use
as selective estrogen receptor modulator
INVENTOR(S): Hoekstra, William Joel; Miller, Aaron Bayne; Zuercher,
William John; Patel, Harikrishna Suryakant
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 42 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082857	A1	20050909	WO 2005-US5467	20050222
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1727802	A1	20061206	EP 2005-723418	20050222
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV				
JP 2007523952	T	20070823	JP 2007-500908	20050222
US 20070203180	A1	20070830	US 2006-598246	20060822

PRIORITY APPLN. INFO.: US 2004-547544P P 20040225
WO 2005-US5467 W 20050222

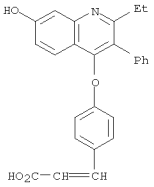
OTHER SOURCE(S): CASREACT 143:266830; MARPAT 143:266830
GI



I

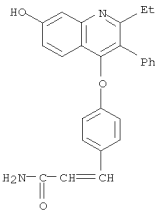
L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

AB The present invention relates to novel compds. of Formula (I, variables defined below) with a variety of therapeutic uses, more particularly novel substituted quinoline compds. particularly useful for selective estrogen receptor modulation. For I, the variables are: R1 = CH=CH-R5; R5 = CN, C(O)OH, C(O)-N(R6)(R7); R6 and R7 = H, alkyl, aryl; or R6 and R7 may combine with the N to which they are attached to form a 3 to 7 membered optionally substituted ring; each R2 independently = H, halogen, haloalkyl, hydroxy, alkoxy, aryloxy, aralkyloxy, alkoxycarbonyloxy, aryloxycarbonyloxy, aralkyloxycarbonyloxy, alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or acyloxy; n = 1 or 2; R3 = H, OH, alkyl, alkoxy, aryloxy, aralkyloxy, haloalkylsulfonyloxy, halogen, haloalkyl, aryl, heteroaryl, aralkyl, or heteroaralkyl; X = O, S, S(O), or S(O)2; each R4 independently = H, halogen, haloalkyl, OH, alkoxy, aryloxy, aralkyloxy, alkoxycarbonyloxy, aryloxycarbonyloxy, aralkyloxycarbonyloxy, alkylsulfonyloxy, arylsulfonyloxy, aralkylsulfonyloxy, or acyloxy; and m = 1 or 2.
IT 828300-07-8P 828300-08-9P 828300-09-0P
828300-10-3P 828300-11-4P 828300-12-5P
828300-13-6P 828300-14-7P 863711-16-4P
863711-17-5P 863711-18-6P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of substituted quinoline compds. for use as selective estrogen receptor modulator to treat various diseases)
RN 828300-07-8 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

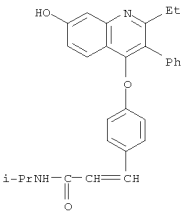


RN 828300-08-9 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(CA INDEX NAME)

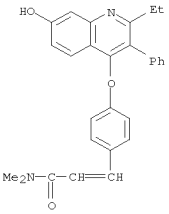


RN 828300-09-0 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N-(1-methylethyl)- (CA INDEX NAME)

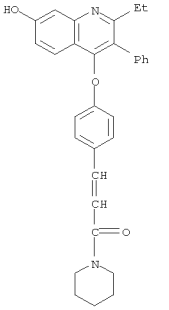


RN 828300-10-3 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N,N-dimethyl- (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

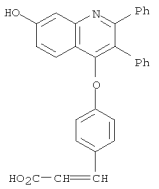


RN 828300-11-4 CAPLUS
CN Piperidine, 1-[3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

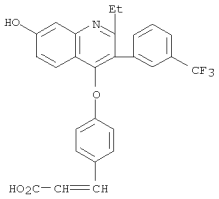


RN 828300-12-5 CAPLUS
CN 2-Propenoic acid, 3-[4-[(7-hydroxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

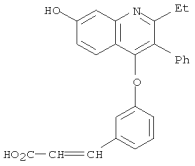


RN 828300-13-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl]oxy]phenyl]- (CA INDEX NAME)

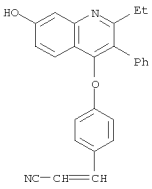


RN 828300-14-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

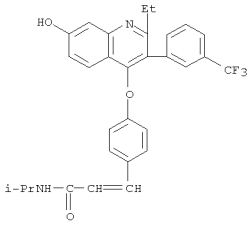


RN 863711-16-4 CAPLUS
CN 2-Propenenitrile, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

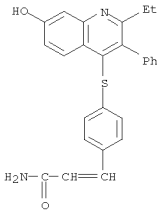


RN 863711-17-5 CAPLUS
CN 2-Propenamide, 3-[4-[[2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl]oxy]phenyl]-N-(1-methylethyl)- (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

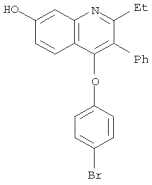


RN 863711-18-6 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)thio]phenyl]- (CA INDEX NAME)

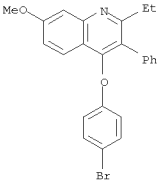


IT 863711-19-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted quinoline compds. for use as selective estrogen
receptor modulator to treat various diseases)
RN 863711-19-7 CAPLUS
CN 7-Quinolinol, 4-(4-bromophenoxy)-2-ethyl-3-phenyl- (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

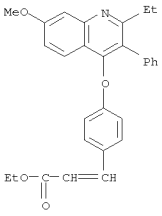


IT 828300-18-1P, 2-Ethyl-3-phenyl-4-(4-bromophenyloxy)-7-methoxyquinoline 828300-22-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted quinoline compds. for use as selective estrogen
receptor modulator to treat various diseases)
RN 828300-18-1 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)



RN 828300-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 4 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

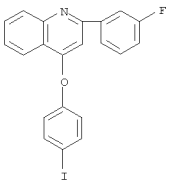
L4 ANSWER 5 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:408026 CAPLUS
Correction of: 2005:155218
DOCUMENT NUMBER: 143:248211
Correction of: 142:197769
TITLE: Product class 3: quinolines
AUTHOR(S): Larsen, R. D.; Cai, D.
CORPORATE SOURCE: Germany
SOURCE: Science of Synthesis (2005), 15, 389-549
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English

AB A review of methods to prepare quinolines including cyclization, ring transformation, aromatization, and substituent modification. The review addnl. covers quinoline 1-oxides and 1-alkyl and 1-arylquinolinium salts.

IT 253433-16-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of quinoline and related derivs. primarily via cyclization,
ring transformation, aromatization and substituent modification methods)

RN 253433-16-8 CAPLUS
CN Quinoline, 2-(3-fluorophenyl)-4-(4-iodophenoxy)- (CA INDEX NAME)



L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:120918 CAPLUS
DOCUMENT NUMBER: 142:219284
TITLE: A preparation of bicyclic imidazole derivatives, useful for the treatment of viral infections mediated by Flaviviridae family of viruses
INVENTOR(S): Schmitz, Franz Ulrich; Roberts, Christopher Don; Griffith, Ronald Conrad; Botyanszki, Janos; Gezginci, Mikail Hakan; Gralapp, Joshua Michael; Shi, Dong Fang;
Liehr, Sebastian J. R.
PATENT ASSIGNEE(S): Genelabs Technologies, Inc, USA
SOURCE: PCT Int. Appl., 327 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005012288	A1	20050210	WO 2004-US24755	20040730
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004261667	A1	20050210	AU 2004-261667	20040730
CA 2534649	A1	20050210	CA 2004-2534649	20040730
US 20050187390	A1	20050825	US 2004-909758	20040730
EP 1651631	A1	20060503	EP 2004-779723	20040730
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1829709	A	20060906	CN 2004-80021754	20040730
BR 2004013234	A	20061003	BR 2004-13234	20040730
JP 2007501189	T	20070125	JP 2006-522111	20040730
MX 2006PA00999	A	20060920	MX 2006-PA999	20060125
IN 2006KN00396	A	20070803	IN 2006-KN396	20060222
NO 2006001013	A	20060428	NO 2006-1013	20060301
PRIORITY APPLN. INFO.:			US 2003-492108P P	20030801
			WO 2004-US24755 W	20040730

OTHER SOURCE(S): CASREACT 142:219284; MARPAT 142:219284
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

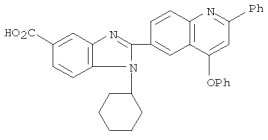
AB The invention relates to a preparation of bicyclic imidazole derivs. of formula

L4 ANSWER 6 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

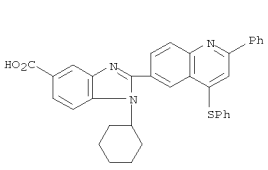
I [wherein: W is CH or N; R is H, (cyclo)alkyl, alk(en/yn)yl, or (hetero)aryl, etc.; X is a fused 6,6-bicycle; Y is halogen, CN, NO2, alkyl, or acyl, etc.; Z is C(O)O-(H/alkyl/alk(en/yn)yl), C(O)NH(alkyl), or
C(O)NH(aryl), etc.], useful for the treatment of viral infections mediated
by Flaviviridae family of viruses. For instance, benzimidazole deriv. II (HCV-NS5b enzyme assay, inhibition data: at 100 μM - 98.22%, at 33 μM - 92.74%) was prepd. via amidation of III by amino acid IV with a yield of 32% (example 4).

IT 841299-19-2P 841299-23-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of bicyclic imidazole derivs. for treatment of viral infections
mediated by Flaviviridae family of viruses)

RN 841299-19-2 CAPLUS
CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-(4-phenoxy-2-phenyl-6-quinolinyl)- (CA INDEX NAME)



RN 841299-23-8 CAPLUS
CN 1H-Benzimidazole-5-carboxylic acid, 1-cyclohexyl-2-[2-phenyl-4-(phenylthio)-6-quinolinyl]- (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

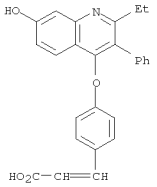
L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1070707 CAPLUS
DOCUMENT NUMBER: 142:212080
TITLE: Discovery of Novel Quinoline-Based Estrogen Receptor Ligands Using Peptide Interaction Profiling
AUTHOR(S): Hoekstra, William J.; Patel, Hari S.; Liang, Xi; Blanc, Jean-Baptiste E.; Heyer, Dennis O.; Willson, Timothy M.; Iannone, Marie A.; Kadwell, Sue H.; Miller, Lisa A.; Pearce, Kenneth H.; Simmons, Catherine A.; Shearin, Jean
CORPORATE SOURCE: GlaxoSmithKline Research Development, Research Triangle Park, NC, 27709-3398, USA
SOURCE: Journal of Medicinal Chemistry (2005), 48(6), 2243-2247
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:212080

AB Traditional approaches to discovery of selective estrogen receptor modulators (SERMs) have relied on ER binding and cell-based estrogen response element-driven assays to identify compds. that are osteoprotective but nonproliferative in breast and uterine tissues. To discover new classes of potential SERMs, we have employed a cell-free microsphere-based binding assay to rapidly characterize ERα interactions with conformation-sensing cofactor or phage display peptides.

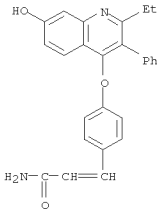
Peptide profiles of constrained triarenes were compared to known proliferative and nonproliferative ER ligands to discover potent quinoline-based ligands with minimal Ishikawa cell stimulation.

IT 828300-07-8P 828300-08-9P 828300-09-0P
828300-10-3P 828300-11-4P 828300-12-5P
828300-13-6P 828300-14-7P 828300-15-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)

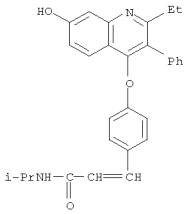
RN 828300-07-8 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



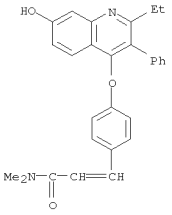
RN 828300-08-9 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



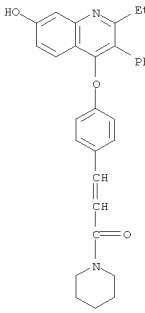
RN 828300-09-0 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N-(1-methylethyl)- (CA INDEX NAME)



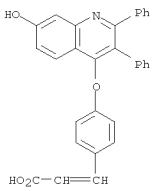
RN 828300-10-3 CAPLUS
CN 2-Propenamide, 3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-N,N-dimethyl- (CA INDEX NAME)



RN 828300-11-4 CAPLUS
CN Piperidine, 1-[3-[4-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]-1-oxo-2-propenyl]- (9CI) (CA INDEX NAME)

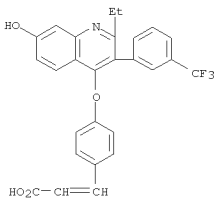


RN 828300-12-5 CAPLUS
CN 2-Propenoic acid, 3-[4-[(7-hydroxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)

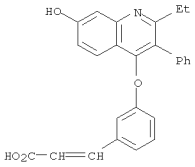


RN 828300-13-6 CAPLUS
CN 2-Propenoic acid, 3-[4-[[2-ethyl-7-hydroxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl]oxy]phenyl]- (CA INDEX NAME)

L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

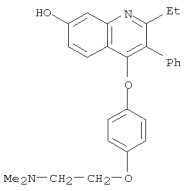


RN 828300-14-7 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-hydroxy-3-phenyl-4-quinolinyl)oxy]phenyl]- (CA INDEX NAME)



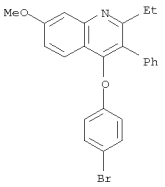
RN 828300-15-8 CAPLUS
CN 7-Quinolinol, 4-[4-[2-(dimethylamino)ethoxy]phenoxy]-2-ethyl-3-phenyl- (CA INDEX NAME)

L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



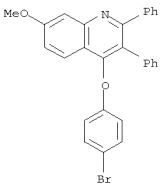
IT 828300-18-1P 828300-19-2P 828300-20-5P
828300-21-6P 828300-22-7P 828300-23-8P
828300-24-9P 828300-25-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(discovery of novel quinoline-based estrogen receptor ligands using peptide interaction profiling)

RN 828300-18-1 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)

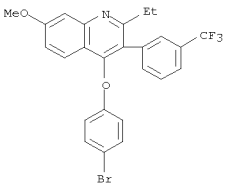


RN 828300-19-2 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-7-methoxy-2,3-diphenyl- (CA INDEX NAME)

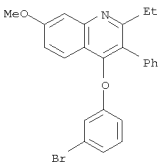
L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-20-5 CAPLUS
CN Quinoline, 4-(4-bromophenoxy)-2-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)

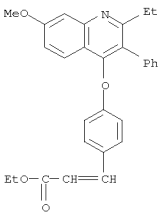


RN 828300-21-6 CAPLUS
CN Quinoline, 4-(3-bromophenoxy)-2-ethyl-7-methoxy-3-phenyl- (CA INDEX NAME)

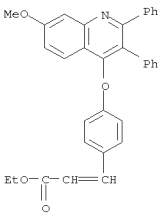


RN 828300-22-7 CAPLUS
CN 2-Propenoic acid, 3-[4-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

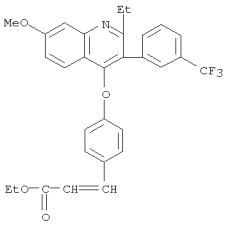


RN 828300-23-8 CAPLUS
CN 2-Propenoic acid, 3-[4-[(7-methoxy-2,3-diphenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)

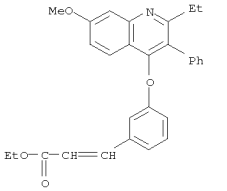


RN 828300-24-9 CAPLUS
CN 2-Propenoic acid, 3-[4-[[2-ethyl-7-methoxy-3-[3-(trifluoromethyl)phenyl]-4-quinolinyl]oxy]phenyl]-, ethyl ester (CA INDEX NAME)

L4 ANSWER 7 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 828300-25-0 CAPLUS
CN 2-Propenoic acid, 3-[3-[(2-ethyl-7-methoxy-3-phenyl-4-quinolinyl)oxy]phenyl]-, ethyl ester (CA INDEX NAME)



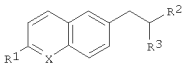
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:892751 CAPLUS
DOCUMENT NUMBER: 139:381384
TITLE: Preparation of 2,6-quinolinyl and 2,6-naphthyl(acylamino)propionic acids as VLA-4 inhibitors
INVENTOR(S): Lassoie, Marie-Agnes; Knerr, Laurent; Demaude, Thierry; De Laveleye, Francoise; Kogej, Thierry; Routier, Sylvain; Guillaumet, Gerald
PATENT ASSIGNEE(S): UCB, S.A., Belg.
SOURCE: PCT Int. Appl., 122 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

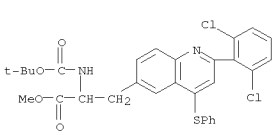
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003093237	A1	20031113	WO 2003-EP3909	20030415
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2484954	A1	20031113	CA 2003-2484954	20030415
AU 2003232472	A1	20031117	AU 2003-232472	20030415
EP 1501801	A1	20050202	EP 2003-747411	20030415
EP 1501801	B1	20080123		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
BR 2003009719	A	20050209	BR 2003-9719	20030415
NZ 536180	A	20050429	NZ 2003-536180	20030415
CN 1649842	A	20050803	CN 2003-809790	20030415
JP 2005535583	T	20051124	JP 2004-501376	20030415
EP 1870402	A1	20071226	EP 2007-17712	20030415
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PT, RO, SE, SI, SK, TR, AL, LT, LV, MK				
RU 2315041	C2	20080120	RU 2004-135304	20030415
AT 384699	T	20080215	AT 2003-747411	20030415
TW 267508	B	20061201	TW 2003-92109709	20030425
ZA 2004008447	A	20060726	ZA 2004-8447	20041019
MX 2004PA10673	A	20050930	MX 2004-PA10673	20041027
NO 2004005234	A	20050118	NO 2004-5234	20041129
US 20080064720	A1	20080313	US 2005-513347	20051121

PRIORITY APPLN. INFO.:
EP 2002-9746 A 20020430
EP 2003-747411 A3 20030415
WO 2003-EP3909 W 20030415

L4 ANSWER 8 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
OTHER SOURCE(S): MARPAT 139:381384
GI

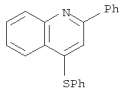


AB Title compds. I [X = N, CH; R1 = R1 = cycloalkyl, aryl, hewterocyclic, heterocyclylalkyl, substituted OH, norbornen-5-yl; R2 = (un)substituted NH2, OH, CONH2; R3 = tetrazolyl, CN, CH2OH, (un)substituted CO2H] were prepared for use in treating VLA-4 dependent inflammatory diseases such as
asthma, allergic rhinitis, sinusitis, conjunctivitis, food allergy, psoriasis, urticaria, pruritus, eczema, rheumatoid arthritis, inflammatory
bowel disease, multiple sclerosis and atherosclerosis (no data). Thus, 4-nitrophenylalanine was esterified, N-protected , reduced to the amine, cyclized with 2,6-Cl2C6H3CHO and CH2:CHSPh, followed by elimination of PhSH to give I [X = N, R1 = 2,6-Cl2C6H3, R2 = NHBoc, R3 = CO2Me]. This compound was deprotected and acylated with 2,6-Cl2C6H3COCl, followed by ester hydrolysis to give I [X = N, R1 = 2,6=Cl2C6H3, R2 = 2,6-Cl2C6H3CONH,
R3 = CO2H].
IT 623147-38-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 2,6-quinolinyl and 2,6-naphthyl(acylamino)propionic acids as
VLA-4 inhibitors)
RN 623147-38-6 CAPLUS
CN 6-Quinolinepropanoic acid, 2-(2,6-dichlorophenyl)-α-[[(1,1-dimethylethoxy)carbonyl]amino]-4-(phenylthio)-, methyl ester (CA INDEX NAME)



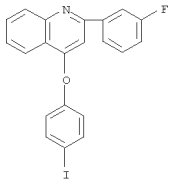
REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:643299 CAPLUS
DOCUMENT NUMBER: 139:276799
TITLE: Use of Highly Active Palladium-Phosphinous Acid Catalysts in Stille, Heck, Amination, and Thiation Reactions of Chloroquinolines
AUTHOR(S): Wolf, Christian; Lerebours, Rachel
CORPORATE SOURCE: Department of Chemistry, Georgetown University, Washington, DC, 20057, USA
SOURCE: Journal of Organic Chemistry (2003), 68(18), 7077-7084
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:276799
AB An efficient synthetic route toward a variety of 2,4-disubstituted quinolines has been developed. Alkylation and arylation of 4-chloroquinoline using organolithium reagents proceed with high regioselectivity in position 2 under cryogenic conditions. The intermediate 1,2-dihydro-4-chloroquinoline derivs. are unstable to air and
are easily oxidized to the corresponding 2-substituted 4-chloroquinolines in high yields. Highly active palladium-phosphinous acid catalysts POPd, POPd1, and POPd2 have been employed in Stille cross-couplings of quinaldine with arylstannanes and in Heck addns. of various 2-substituted 4-chloroquinolines to tert-Bu acrylate. In particular, POPd combines high
catalytic activity for cross-coupling reactions with simplicity of use due
to its stability to air. Utilizing CsF in POPd-catalyzed Stille couplings
further increased the reactivity of arylstannanes, which was attributed to
the fluorophilicity of organotin compds. Basic additives were found to exhibit a significant effect on the yields of the POPd-promoted Heck reactions. In general, dicyclohexylmethylamine affords superior results than NaOAc, Cs2CO3, or t-BuOK. POPd was also found to tolerate amine and thiol substrates and proved to promote carbon-heteroatom bond formation of
chloroquinoline derivs. with aliphatic and aromatic amines and thiols, resp.
IT 606125-62-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Stille, Heck, amination, and thiation reactions of chloroquinolines in
presence of palladium-phosphinous acid catalysts)
RN 606125-62-6 CAPLUS
CN Quinoline, 2-phenyl-4-(phenylthio)- (CA INDEX NAME)



L4 ANSWER 9 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
REFERENCE COUNT: 80 THERE ARE 80 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:709981 CAPLUS
DOCUMENT NUMBER: 132:64150
TITLE: Synthesis of functionalized quinolines through tandem addition/annulation reactions of β-(2-aminophenyl)-α,β-ynones
AUTHOR(S): Arcadi, Antonio; Marinelli, Fabio; Rossi, Elisabetta
CORPORATE SOURCE: Dipartimento di Chimica Ingegneria Chimica e Materiali della Facolta di Scienze, Universita di L'Aquila, L'Aquila, I-67100, Italy
SOURCE: Tetrahedron (1999), 55(46), 13233-13250
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 132:64150
AB β-(2-Aminophenyl)-α,β-ynones can quickly give functionalized 2,4-disubstituted quinolines through tandem nucleophilic addition/annulations reactions. Acid-catalyzed cyclization of β-(2-aminophenyl)-α,β-ynones can also occur. The easy entry into 4-iodo-2-substituted quinolines prompted the development of a one pot procedure for synthesis of 2,4-disubstituted quinolines by further elaboration by means of palladium-catalyzed reactions. The exposure to basic conditions of one β-(2-malonylamidophenyl)-α,β-ynone led to a fused quinolone derivative through intramol. Michael addition/tautomerization/transesterification cascade reactions. Fused polycyclic quinolines can be viewed as occurring through a tandem concerted Diels-Alder/annulation reactions of β-(2-aminophenyl)-α,β-ynones with enamines, azides and nitrile oxides.
IT 253433-16-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of functionalized quinolines through tandem addition/annulation reactions of β-(2-aminophenyl)-α,β-ynones)
RN 253433-16-8 CAPLUS
CN Quinoline, 2-(3-fluorophenyl)-4-(4-iodophenoxy)- (CA INDEX NAME)



L4 ANSWER 10 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

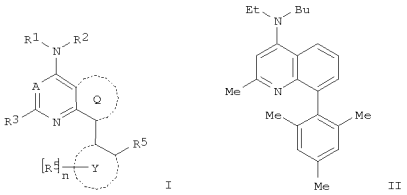
L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:194128 CAPLUS
DOCUMENT NUMBER: 130:237583
TITLE: Preparation of quinoline and quinazoline derivatives having corticotropin releasing factor (CRF) antagonist activity
INVENTOR(S): Den Hartog, Jacobus A. J.; Visser, Gerben M.; Toorop, Gerrit P.; Jansen, Johannes W. C. M.; Ronken, Eric; Tulp, Martinus T. M.; Reinders, Jan H.
PATENT ASSIGNEE(S): Duphar International Research B.V., Neth.
SOURCE: PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9912908	A1	19990318	WO 1998-EP5726	19980907
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
NL 1010018	C2	19990310	NL 1998-1010018	19980904
CA 2270777	A1	19990318	CA 1998-2270777	19980907
AU 9896241	A	19990329	AU 1998-96241	19980907
EP 966442	A1	19991229	EP 1998-950008	19980907
EP 966442	B1	20061220		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY				
JP 2001505226	T	20010417	JP 1999-515100	19980907
AT 348812	T	20070115	AT 1998-950008	19980907
US 6350750	B1	20020226	US 1999-297837	19990913

PRIORITY APPLN. INFO.: EP 1997-202762 A 19970909
WO 1998-EP5726 W 19980907

OTHER SOURCE(S): MARPAT 130:237583
GI

L4 ANSWER 11 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



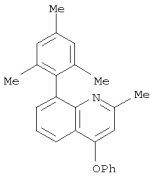
I II

AB The title compds. [I; A = CH, N; Q = (un)substituted Ph, pyridyl, pyrimidinyl, pyridazinyl; Y = Ph, pyridyl, pyrimidinyl, etc.; R1, R2 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R3 H, alkyl optionally substituted with one or more F atoms; R4 = halo, MeO, EtO, etc.; R5 = halo, alkyl, alkenyl, etc.; n = 0-4], having corticotropin releasing factor (CRF) antagonist activity (no data) and useful in the treatment of a wide range of stress related disorders, were prepared E.g., a 4-step synthesis of quinoline II, starting with 2-methyl-4-hydroxy-8-bromoquinoline, was given.

IT 221298-72-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinoline and quinazoline derivs. having corticotropin releasing factor (CRF) antagonist activity)

RN 221298-72-2 CAPLUS

CN Quinoline, 2-methyl-4-phenoxy-8-(2,4,6-trimethylphenyl)- (CA INDEX NAME)



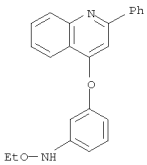
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN 220412-52-2 CAPLUS

CN Benzenamine, N-ethoxy-3-[(2-phenyl-4-quinolinyl)oxy]- (CA INDEX NAME)



REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L4 ANSWER 12 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1999:1983 CAPLUS

DOCUMENT NUMBER: 130:162747

TITLE: Quantitative structure-activity relationship studies on some nonbenzodiazepine series of compounds acting at the benzodiazepine receptor

AUTHOR(S): Gupta, S. P.; Paleti, Anitha

CORPORATE SOURCE: Department of Chemistry, Birla Institute of Technology

and Science, Pilani, 333 031, India

SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(11), 2213-2218

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB QSAR studies were carried out on a few non-benzodiazepine series of compds. such as 3-substituted-imidazo[1,2-b]pyridazines, 2-phenylimidazo[1,2-α]pyridines, 2-(alkoxycarbonyl)imidazo[2,1-b]benzothiazoles, and 2-arylquinolines. For the first series of compds. a

Fujita-Ban approach was followed, which revealed the highest activity contribution for 3,4-OCH2O group of 2-Ph moiety and for a methoxy group at

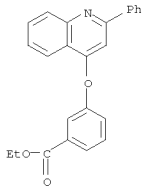
6-position. For the rest of the series, a Hansch approach has been adopted. The hydrophobic and electronic properties of the various substituents had major roles in the binding of these compds. with the receptor. Based on these studies, a hypothetical model for the drug-receptor interaction has been proposed.

IT 178990-56-2 220412-52-2
RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); PRP (Properties); BIOL (Biological study)
(QSAR of nonbenzodiazepine imidazo-heterocycles and quinolines acting at benzodiazepine receptor)

RN 178990-56-2 CAPLUS

CN Benzoic acid, 3-[(2-phenyl-4-quinolinyl)oxy]-, ethyl ester (CA INDEX NAME)



L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1998:160490 CAPLUS

DOCUMENT NUMBER: 128:243967

TITLE: Silane-mediated direct condensation of nitroarenes with cinnamyl-type sulfones. The way to 2-aryl-4-X-quinolines and their hetero analogs

AUTHOR(S): Wrobel, Zbigniew

CORPORATE SOURCE: Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, PL-01-224, Pol.

SOURCE: Tetrahedron (1998), 54(11), 2607-2618

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

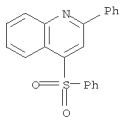
OTHER SOURCE(S): CASREACT 128:243967

AB DBU/silane mediated double condensation of nitroarenes with cinnamyl-type sulfones proceeds smoothly to yield 2-aryl-4-arylsulfonyl quinolines and their hetero analogs. Arylsulfonyl group can be easily replaced by different nucleophiles.

IT 64495-62-1P 204913-34-8P 204913-36-0P
204913-37-1P 204913-38-2P 204913-39-3P
204913-40-6P 204913-41-7P 204913-42-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

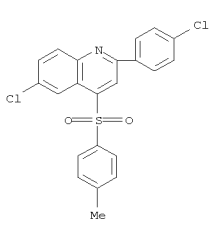
RN 64495-62-1 CAPLUS

CN Quinoline, 2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)

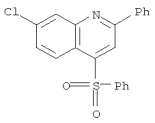


RN 204913-34-8 CAPLUS

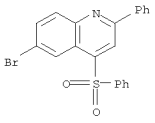
CN Quinoline, 6-chloro-2-(4-chlorophenyl)-4-[(4-methylphenyl)sulfonyl]- (CA INDEX NAME)



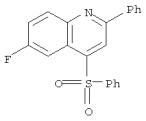
L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
RN 204913-36-0 CAPLUS
CN Quinoline, 7-chloro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



RN 204913-37-1 CAPLUS
CN Quinoline, 6-bromo-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



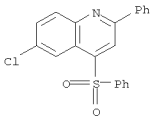
RN 204913-38-2 CAPLUS
CN Quinoline, 6-fluoro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



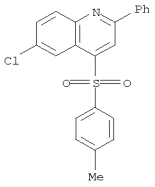
RN 204913-39-3 CAPLUS
CN Quinoline, 6-(methylsulfonyl)-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)

L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

IT 204913-33-7P 204913-35-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of (aryl)quinolines via silane-mediated condensation of nitroarenes with cinnamyl-type sulfones)
RN 204913-33-7 CAPLUS
CN Quinoline, 6-chloro-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)

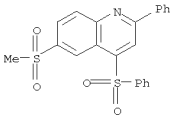


RN 204913-35-9 CAPLUS
CN Quinoline, 6-chloro-4-[(4-methylphenyl)sulfonyl]-2-phenyl- (CA INDEX NAME)

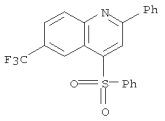


REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

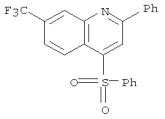
L4 ANSWER 13 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



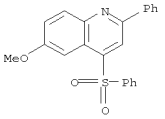
RN 204913-40-6 CAPLUS
CN Quinoline, 2-phenyl-4-(phenylsulfonyl)-6-(trifluoromethyl)- (CA INDEX NAME)



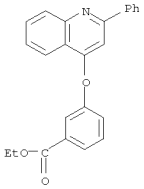
RN 204913-41-7 CAPLUS
CN Quinoline, 2-phenyl-4-(phenylsulfonyl)-7-(trifluoromethyl)- (CA INDEX NAME)



RN 204913-42-8 CAPLUS
CN Quinoline, 6-methoxy-2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)

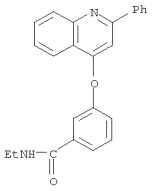


L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:380980 CAPLUS
DOCUMENT NUMBER: 125:104254
TITLE: Oxadiazoles as bioisosteric transformations of carboxylic functionalities. II
AUTHOR(S): Andersen, K. E.; Lundt, B. F.; Joergensen, A. S.; Braestrup, C.
CORPORATE SOURCE: Novo Nordisk A/S, Naaloev, 2760, Den.
SOURCE: European Journal of Medicinal Chemistry (1996), 31(5),
417-425
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:104254
AB To improve the in vivo efficacy of a series of known benzodiazepine receptor (BZR) ligands, 1-(2-phenyl-4-quinolinyl)-4-piperinecarboxamides, a series of analogs has been prepared in which the amide group of these ligands has been replaced by a 1,2,4-oxadiazole moiety or converted to other carboxylic isosters such as esters or nitriles. An increase in the in vivo efficacy was observed for some of the compds. prepared in this investigation compared to the parent carboxamide derivs.
IT 178990-56-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of 1-(2-phenyl-4-quinolinyl)-4-piperidinecarboxamides analogs
as benzodiazepine receptor ligands)
RN 178990-56-2 CAPLUS
CN Benzoic acid, 3-[(2-phenyl-4-quinolinyl)oxy]-, ethyl ester (CA INDEX NAME)



IT 178990-57-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 1-(2-phenyl-4-quinolinyl)-4-piperidinecarboxamides analogs

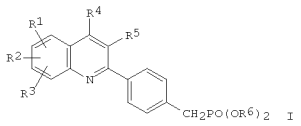
L4 ANSWER 14 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
as benzodiazepine receptor ligands)
RN 178990-57-3 CAPLUS
CN Benzamide, N-ethyl-3-[(2-phenyl-4-quinolinyl)oxy]- (CA INDEX NAME)



L4 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:495360 CAPLUS
DOCUMENT NUMBER: 119:95360
TITLE: Preparation of quinolines as hypolipemics and antidiabetics
INVENTOR(S): Myata, Kazuyoshi; Shoji, Yasuo; Tsuda, Yoshihiko; Tsutsumi, Kazuhiko; Kamisaka, Eiji; Inoe, Yasuhide
PATENT ASSIGNEE(S): Otsuka Pharma Co Ltd, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

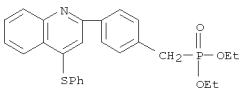
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05043589	A	19930223	JP 1992-13186	19920128
PRIORITY APPLN. INFO.:			JP 1991-102184	A1 19910205

OTHER SOURCE(S): MARPAT 119:95360
GI



AB The title compds. I [R1-R3 = H, lower alkyl, lower alkoxy, halo, NO2; R4, R5 = H, lower alkyl, (halo-substituted) Ph, PhS, OH, cyano, lower alkoxycarbonyl, halo; R6 = lower alkyl], useful as hypolipemics and antidiabetics (no data), are prepared Refluxing 49.0 g 6-chloro-2-(4-methylphenyl)-4-phenylquinoline with NBS and Bz2O2 in C6H6 for 15 h gave 24.0 g 2-(4-bromomethylphenyl)-6-chloro-4-phenylquinoline, which (10.3 g) was treated with tri-Et phosphite at 160° for 1 h to afford 7.3 g I (R1 = 6-Cl, R2 = R3 = R5 = H, R4 = Ph, R6 = Et).
IT 149193-10-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as hypolipemic and antidiabetic agent)
RN 149193-10-2 CAPLUS
CN Phosphonic acid, [[4-[4-(phenylthio)-2-quinolinyl]phenyl]methyl]-, diethyl
ester (9CI) (CA INDEX NAME)

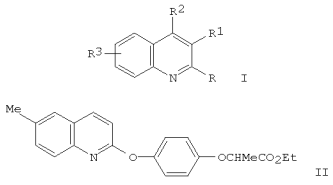
L4 ANSWER 15 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:598123 CAPLUS
DOCUMENT NUMBER: 97:198123
ORIGINAL REFERENCE NO.: 97:33181a,33184a
TITLE: Quinolineoxyphenoxypropionic acid derivatives and their use as herbicides
INVENTOR(S): Mildenberger, Hilmar; Knorr, Harald; Bauer, Klaus
PATENT ASSIGNEE(S): Hoechst A.-G. , Fed. Rep. Ger.
SOURCE: Ger. Offen., 20 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

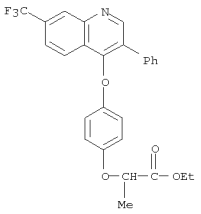
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3101544	A1	19820819	DE 1981-3101544	19810120
PRIORITY APPLN. INFO.:			DE 1981-3101544	19810120

OTHER SOURCE(S): CASREACT 97:198123
GI

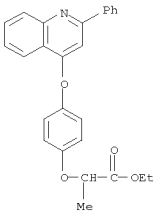


AB I [one of R or R2, especially R = 4-R4CHMeOC6H4O(R4 = CO2H or a derivative, e.g.
amide) and the other = H, C1-4 alkyl, Ph, Cl, Br; R1 = H, C1-4 alkyl, Cl, Br, cyano, C1-4 carbalkoxy; R3 = H, C1-4 alkyl alkoxy, or dialkylamino, NO2, CF3, halo; n = 0-2] were prepared as herbicides. Thus, 21 g 4-HOC6H4OCHMeCO2Et were added dropwise to 2.9 g NaH in 100 mL DMF, 17.7 g 2-chloro-6-methylquinoline added, and the mixture was stirred 2 h at 100° to give 89.2% II.
IT 83596-68-3P 83596-71-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)
RN 83596-68-3 CAPLUS
CN Propanoic acid, 2-[4-[[3-phenyl-7-(trifluoromethyl)-4-quinolinyl]oxy]phenoxy]-, ethyl ester (CA INDEX NAME)

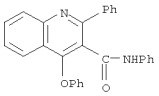
L4 ANSWER 16 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



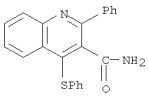
RN 83596-71-8 CAPLUS
CN Propanoic acid, 2-[4-[(2-phenyl-4-quinolinyl)oxy]phenoxy]-, ethyl ester (CA INDEX NAME)



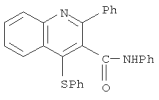
L4 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



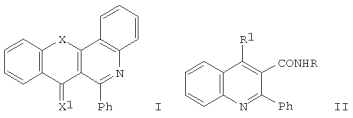
RN 65031-30-3 CAPLUS
CN 3-Quinolinecarboxamide, 2-phenyl-4-(phenylthio)- (CA INDEX NAME)



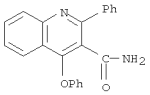
RN 65031-32-5 CAPLUS
CN 3-Quinolinecarboxamide, N,2-diphenyl-4-(phenylthio)- (CA INDEX NAME)



L4 ANSWER 17 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:22706 CAPLUS
DOCUMENT NUMBER: 88:22706
ORIGINAL REFERENCE NO.: 88:3645a,3648a
TITLE: Synthesis and structure of some new heterocyclic analogs of benzanthracene
AUTHOR(S): Bala, Marian
CORPORATE SOURCE: Inst. Chem., Jagellonian Univ., Krakow, Pol.
SOURCE: Zeszyty Naukowe Uniwersytetu Jagiellonskiego, Prace Chemiczne (1976), 21, 171-7
CODEN: ZUJCAQ; ISSN: 0373-0166
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

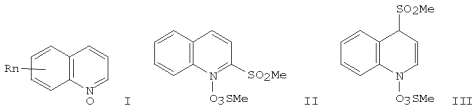


AB Condensed quinolines I (X = O, S, X1 = O) were obtained by treating II (R = H, R1 = Cl) with PhXH, and cyclizing II (R = H, R1 = XPh) with polyphosphoric acid. Treatment of II (R = Ph, R1 = Cl) with PhXH and cyclization of II (R = Ph, R1 = XPh) gave I (X = O, S, X1 = NPh), which were hydrolyzed to I (X1 = O).
IT 65031-26-7P 65031-28-9P 65031-30-3P
65031-32-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclization of)
RN 65031-26-7 CAPLUS
CN 3-Quinolinecarboxamide, 4-phenoxy-2-phenyl- (CA INDEX NAME)

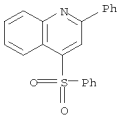


RN 65031-28-9 CAPLUS
CN 3-Quinolinecarboxamide, 4-phenoxy-N,2-diphenyl- (CA INDEX NAME)

L4 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1977:567846 CAPLUS
DOCUMENT NUMBER: 87:167846
ORIGINAL REFERENCE NO.: 87:26519a,26522a
TITLE: The reaction of heteroaromatic N-oxide with acid chloride and cyanide. The reaction of quinoline N-oxides with sulfonic acid chloride and potassium cyanide
AUTHOR(S): Hayashi, Eisaku; Shimada, Noriaki
CORPORATE SOURCE: Shizuoka Coll. Pharm., Shizuoka, Japan
SOURCE: Yakugaku Zasshi (1977), 97(6), 627-40
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
GI

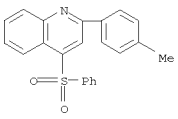


AB Reaction of 17 quinoline oxides I (e.g., Rn = H, Me, MeO, Ph, CN, halo) with ClSO2Me and KCN gave the 2-(methylsulfonyl)quinolines or, when the 2-position was substituted, the 4-(methylsulfonyl) derivs. via elimination
of HO3SMe from the intermediates II or III.
IT 64495-62-1P 64495-63-2P
RL: PREP (Preparation)
(by reaction of quinoline oxide derivative with sulfonic acid chloride)
RN 64495-62-1 CAPLUS
CN Quinoline, 2-phenyl-4-(phenylsulfonyl)- (CA INDEX NAME)



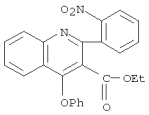
RN 64495-63-2 CAPLUS
CN Quinoline, 2-(4-methylphenyl)-4-(phenylsulfonyl)- (CA INDEX NAME)

L4 ANSWER 18 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



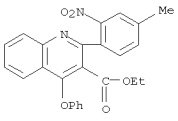
L4 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1971:53602 CAPLUS
DOCUMENT NUMBER: 74:53602
ORIGINAL REFERENCE NO.: 74:8637a,8640a
TITLE: Cyclic amidines. XXIII. Dibenzo[b,h][1]benzopyrano[2,3,4-de][1,6]naphthyridines and their molecular orientation in carcinogenesis
AUTHOR(S): Partridge, Maurice W.; Bloomfield, D. G.; Vipond, H. J.
CORPORATE SOURCE: Univ. Nottingham, Nottingham, UK
SOURCE: Journal of the Chemical Society [Section] C: Organic (1970), (19), 2647-53
CODEN: JSOOAX; ISSN: 0022-4952
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB Cyclizations of substituted dibenzo[b,h][1,6]naphthyridines and of substituted [1]benzopyrano[3,2-c]quinolin-7-ones, and the condensation of N-carboxyanthranilic acid anhydrides with substituted 1,3-diphenylpropane-1,3-diones followed by a reductive cyclization, leading unequivocally to dibenzo[b,h][1]benzopyrano[2,3,4-de]-[1,6]naphthyridine (I) and five isomeric Me derivs., are described. An explanation is given of the differences in carcinogenic activity of the 2-, 7-, and 12-methyl derivs. consistent with specific mol. orientations for carcinogenesis similar to those deduced for tricycloquinazoline and its derivs.
IT 30413-10-6P 30413-11-7P 30413-12-8P 30413-13-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 30413-10-6 CAPLUS
CN 3-Quinolinecarboxylic acid, 2-(o-nitrophenyl)-4-phenoxy-, ethyl ester (8CI) (CA INDEX NAME)

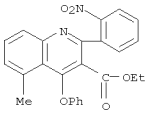


RN 30413-11-7 CAPLUS
CN 3-Quinolinecarboxylic acid, 2-(2-nitro-p-tolyl)-4-phenoxy-, ethyl ester (8CI) (CA INDEX NAME)

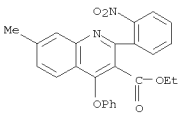
L4 ANSWER 19 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 30413-12-8 CAPLUS
CN 3-Quinolinecarboxylic acid, 5-methyl-2-(o-nitrophenyl)-4-phenoxy-, ethyl ester (8CI) (CA INDEX NAME)



RN 30413-13-9 CAPLUS
CN 3-Quinolinecarboxylic acid, 7-methyl-2-(o-nitrophenyl)-4-phenoxy-, ethyl ester (8CI) (CA INDEX NAME)



L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:25581 CAPLUS
DOCUMENT NUMBER: 52:25581
ORIGINAL REFERENCE NO.: 52:4658f-i,4659a-i
TITLE: Triazaphenanthrenes. II. Derivatives of 10-phenyl-1,2,9-triazaphenanthrene
AUTHOR(S): Atkinson, C. M.; Mattocks, A. R.
SOURCE: Journal of the Chemical Society (1957) 3722-6
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:25581
AB A preparative route to 4-acetyl-3-amino-2-phenylquinoline (I) was developed. Diazotization of I in HCl and subsequent cyclization gave chiefly 4-acetyl-3-chloro-2-phenylquinoline (II), with 10% of the hydroxytriazaphenanthrene (III); an 80% yield of III was obtained by cyclization in an alkaline medium. 4-Amino-10-phenyl-1,2,9-triazaphenanthrene (IV) formed a monomethiodide (V) which was biologically inactive. 2-Phenyl-3-phthalimidoquinoline-4-carboxylic acid (VI) (40 g.) refluxed 0.5 hr. with 400 cc. 50% volume/volume H_2SO_4 gave 3-amino-2-phenylquinoline (VII), m. 119°. Neutralization of the mother liquors and reextn. with $CHCl_3$ gave 3-amino-2-phenylquinoline-4-carboxylic acid (VIII), m. 224°. VI was recovered after 2 hrs. heating with 20% or 75% NaOH. VII was also formed by similar treatment of 2-phenyl-3-phthalimidoquinoline (IX). VI (2.5 g.) and 15 cc. H_3PO_4 heated 1 hr. at 215° gave IX, m. 249-50° (C_6H_6). The presence of VII in the aqueous mother liquors was indicated by its fluorescence and by the sublimate of phthalic anhydride in the condenser. VII (18 g.) in 45 cc. H_2O and 75 cc. concentrated HCl diazotized at 0° with 6 g. $NaNO_2$, the solution treated at 0° in 54 g. $SnCl_2$ and 54 cc. concentrated HCl and 100 cc. H_2O, the mixture kept 0.5 hr. at 0°, allowed to come to room temperature overnight, diluted to 1500 cc., partially neutralized with 25 g. NaOH in 50 cc. H_2O, the Sn salts removed as the sulfide, and the precipitate collected, then digested with refluxing H_2O, the combined filtrates concentrated to 350 cc., and then cooled gave 3-hydrazino-2-phenylquinoline-HCl (X), m. 255° (decomposition). The hydrazone of EtAc (XI) (16 cc.) prepared from 10 g. of X by refluxing 5 min. with 16 g. NaOAc in 16 cc. H_2O and 25 cc. alc. in 9.3 g. yield, m. 123° (aqueous alc.). The derivative (XIa) from PhCOEt, prepared by the same method, was a sticky solid which could not be crystallized XI (9.3 g.) heated 6 hrs. with 80 cc. concentrated HCl gave 5.9 g. 4',5'-dimethyl-2-phenylpyrrolo-[2',3'-3,4]quinoline (XII).HCl, m. about 300° (variable). XII.HCl made alkaline with NH_3 gave free XII, needles, m. 304-5° (C_6H_6). XII was recovered unchanged after 4.5 hrs. heating with either AcCl or Ac_2O. Crude XIa (2.8 g.) heated 6 hrs. with 30 cc. concentrated HCl gave 4'-methyl-2,5'-diphenylpyrrolo-[2',3'-3,4]quinoline-HCl, m. about 300° (variable). VI (10 g.) refluxed 0.5 hr. with 30 cc. $SOCl_2$ and then heated 0.5 hr. with 50 cc. alc. gave Et 2-phenyl-3-phthalimidoquinoline-4-carboxylate, leaflets, m. 192-3°

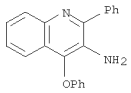
L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(alc.). VI (50 g.) refluxed 0.5 hr. with 75 cc. SOCl2 and the acid chloride suspended in dry C6H6 stirred 18 hrs. with a suspension of Na malonic acid ester [from 24 cc. CH2(CO2Et)2, 4.2 g., and 200 cc. C6H6], the mixt. refluxed 5 hrs., stirred 18 hrs. at room temp., heated to about 60° and stirred 0.25 hr. with 60 cc. concd. HCl in 100 cc. H2O, and the aq. layer extd. with C6H6 gave a condensation product. This substance (15 g.) refluxed 10 min. with 210 cc. 35% H2SO4 gave 10 g. 4-acetyl-2-phenyl-3-phthalimidoquinoline (XIII), m. 240-1° (alc.); oxime, m. 240° (decompn.). XIII (3 g.) heated 4 hrs. with 20 cc. AcOH and 3 cc. 100% N2H4.H2O gave the hydrazone, orange powder, m. 196° (decompn.). XIII (0.5 g.) refluxed 3.5 hrs. with 8 cc. 48% HBr and the filtrate basified gave VII. VIII (2 g.) refluxed 0.5 hr. with 5 cc. SOCl2 and the residue left a few hrs. at room temp. with 20 cc. 15% HCl and the filtrate made alk. gave 3-amino-4-chloro-2-phenylquinoline (XIV), needles, m. 126° (ligroine); acetyl deriv, m. 195° (C6H6). An identical expt. in which the HCl treatment was omitted, yielded by digestion with ligroine a small amt. of a solid which spontaneously decompd. with evolution of SO2. The compd., m. 126°, was unchanged after refluxing 2 hrs. with 18% H2SO4, but 1 hr. with 55% H2SO4 gave 3-amino-4-hydroxy-2-phenylquinoline, m. 251° (decompn.). XIV (0.5 g.) in 7 g. PhOH treated 1.5 hr. at 195° with dry NH3, the mixt. treated with 100 cc. H2O and NaOH soln., and isolated gave 0.3 g. 3-amino-4-phenoxy-2-phenylquinoline (XV), m. 175°. Treatment of XIV with PhOH and KOH at 100° failed to provide XV. Attempts to convert XV into the 4-amino deriv. by heating with NH4OAc at 140° failed. 3-Amino-4-cyano-2-phenylquinoline (24 g.) added during 0.5 hr. to MeMgI (from 20 cc. MeI) in 150 cc. Et2O and 450 cc. C6H6, the mixt. refluxed 20 hrs., stirred with 1400 g. ice and 360 cc. concd. HCl, the org. layer extd. with 5N HCl, the acid portion basified, extd. with C6H6 gave 22.4 g. ketimine (XVI), m. 133-4° (C6H6-ligroine). XVI (15 g.) refluxed 1 hr. with H2O and concd. HCl gave I, needles, m. 93-4° (hexane). 3-Amino-2-phenylquinoline-4-carboxamide (35 g.) refluxed 3.5 hrs. with MeMgI (from 54 cc. MeI) gave 29 g. XVI which was then hydrolyzed to 25 g. almost pure I. I (12 g.) in 30 cc. concd. HCl and 120 cc. H2O cooled to -5° and treated during 5 min. with 3.1 g. NaNO2 in 65 cc. H2O, then set aside 2 hrs. at room temp. gave III, plates, m. 262° (alc.). I (1 g.) treated 5 min. in 25 cc. concd. HCl at 0° with 0.3 g. NaNO2 in H2O, after a few min. 75 cc. concd. HCl added, and the mixt. heated 4 hrs. at 60° and isolated gave 90 mg. III and II, m. 100-1°. III (11 g.), 17 g. PCl5, and 85 cc. POCl3 refluxed 2.5 hrs., the POCl3 removed, the residue shaken 20 min. with 100 cc. C6H6, 150 g. ice, and 100 cc. 3N NaOH gave 9.4 g. 4-chloro-10-phenyl-1,2,9-triazaphenanthrene (XVII), blades, m. 186° (EtOAc). Dry NH3 was passed through 0.4 g. XVII in 2 g. PhOH at 180°, the mixt. heated 15 min. with 4 g. NaOH in 30 cc. H2O, and the product isolated gave 0.4 g. 4-phenoxy-10-phenyl-1,2,9-triazaphenanthrene (XVIII), pink needles, m. 221°. XVII (6 g.) heated 1.5 hrs. with 2 g. KOH in 30 g. PhOH and digested with 350 cc. warm 1.5N NaOH gave 8 g. XVIII. XVIII (1 g.)

L4 ANSWER 20 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
heated 3 hrs. with 10 g. NH4OAc at 180-200° and then digested with dil. NaOH gave 0.45 g. IV, m. 276° (MeNO2). A stream of dry NH3 passed 0.5 hr. into a soln. of 0.5 g. XVIII in 5 g. AcNH2 at 175° gave 0.3 g. of a product which contained 50 mg. IV; 4-acetate, m. 287-9° (AcOH). IV (1.2 g.) refluxed 2 hrs. with MeI in 10 cc. MeOH gave 0.9 g. V, m. 285° (decompn.). III (1 g.) in 10 cc. 3N NaOH treated 5 min. at 55° with 1 cc. Me2SO4 gave 0.7 g. N'-methyl-4-oxo-10-phenyl-1,2,9-triazaphenanthrene, m. 280-1° (BuOH). XVII (0.6 g.) refluxed 2 hrs. with MeOH-NaOMe gave 4-methoxy-10-phenyl-1,2,9-triazaphenanthrene, needles, m. 194-8° (alc.).

IT 102241-29-2P, Quinoline, 3-amino-4-phenoxy-2-phenyl-
RL: PREP (Preparation)
(preparation of)

RN 102241-29-2 CAPLUS

CN Quinoline, 3-amino-4-phenoxy-2-phenyl- (6CI) (CA INDEX NAME)



L4 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1958:25580 CAPLUS

DOCUMENT NUMBER: 52:25580

ORIGINAL REFERENCE NO.: 52:4657g-i,4658a-f

TITLE: Triazaphenanthrenes. I. Derivatives of 10-phenyl-1,3,9-triazaphenanthrene

AUTHOR(S): Atkinson, C. M.; Mattocks, A. R.

SOURCE: Journal of the Chemical Society (1957) 3718-21
CODEN: JCSOA9; ISSN: 0368-1769

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

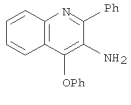
AB Various 4-substituted derivs. of 10-phenyl-1,3,9-triazaphenanthrene (I) were prepared Monomethiodides of the compds. were found to be biol. inactive. Attempts to prepare an N-oxide yielded only OH compds. PhAc (200 g.) and 86 cc. Br gave 60% PhCOCH2Br (II). Phenacylphthalimide (54 g.) in 200 cc. hot alc. mixed with 40 g. KOH in 40 cc. H2O added to 30 g. isatin in 200 cc. alc. containing 25 g. KOH in 15 cc. H2O, another lot of 25 g. KOH in 50 cc. H2O added, and the solution left 3 days, the mixture neutralized with concentrated HCl, and the product isolated gave 2-phenyl-3-phthalimidoquinoline-4-carboxylic acid (III), m. 278° (decomposition) (dioxane). N2H4.H2O (40 cc.) and 80 g. III refluxed 0.5 h. in 300 cc. AcOH, 1,4-dihydroxyphthalazine, m. about 340°, separating on cooling, the filtrate concentrated and set aside at 0°, and the product isolated gave 32 g. 3-amino-2-phenylquinoline-4-carboxylic acid (IV), m. 223-4° (dioxane); acetyl derivative, m. 271° (decomposition). IV (105 g.) refluxed 15 min. with 300 cc. SOCl2 and the product dissolved in 1250 cc. C6H6, a stream of dry NH3 passed in for 0.5 h., and the product collected after concentration gave 2-phenyl-3-phthalimidoquinoline-4-carboxamide (V), m. 343° (AcOH). V (112 g.) refluxed 2 h. with 200 cc. N2H4.H2O and 400 cc. C5H5N gave 3-amino-phenyl-quinoline-4-carboxamide (VI), needles, m. 265° (MeOH). VI (50 g.) and 125 g. P2O5 heated 1 h. at 175°, then added to ice and H2O, and the mixture made alkaline gave 3-amino-4-cyano-2-phenylquinoline (VII), m. 194° (C6H6). IV (15 g.) refluxed 1 h. with 25 cc. HCONH2 gave 4-hydroxy-10-phenyl-1,3,9-triazaphenanthrene (VIII), m. 307-8° (dioxane). VIII (7 g.) and 11.5 g. PCl5 heated 22 h. at 150-60° in a sealed tube, the product removed with hot C6H6, shaken 15 min. with 100 cc. 6N NaOH, and the product isolated gave 7.2 g. 4-chloro-10-phenyl-1,3,9-triazaphenanthrene (IX), needles, m. 167-8° (EtOAc or ligroine). The use of refluxing POCl3, alone or with PCl5, did not give the desired product. IX (5 g.) and 20 g. PhOH treated 1.25 h. at 180° with passage of NH3 and the mixture heated 0.5 h. on the steam bath with 120 cc. 3N NaOH gave 4.6 g. 4-amino-10-phenyl-1,3,9-triazaphenanthrene (X), blades, m. 233-4° (C6H6). VII (10 g.) and 70 cc. HCONH2 refluxed 1 h. gave 3.15 g. X as platelets (EtOAc). X was prepared in lower yield by heating IX with CO(NH2)2 44 h. at 190° in a sealed tube. The 4-phenoxy compound (XI) (50 mg.) heated 0.5 h. at 180° with 1 g. NH4OAc gave X; acetyl derivative, m. 251-2° (AcOH); MeI salt, needles, m. 239° (decomposition), and concentration of the liquors gave another salt, m. 216° (decomposition), of which there was insufficient for anal. IX (1 g.) heated 1.5 h. in 5 g. PhOH containing 0.25 g. KOH and then shaken 0.5 h. with 60 cc.

L4 ANSWER 21 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
1.5N NaOH gave 1 g. XI, m. 193-4° (C6H6). IX (9.3 g.) refluxed 2.5 h. with 11.6 g. p-toluenesulfonylhydrazide in 220 cc. dry CHCl3 gave an intermediate which, added portionwise to 200 cc. N NaOH, then left 0.5 h., gave on crystn. 4.2 g. I, m. 174-5.5° (ligroine). I (2.6 g.) heated 10 min. at 100° with 15 cc. Me2SO4, the mixt. dissolved in 50 cc. warm H2O, shaken with C6H6, and the aq. layer treated with 15 cc. satd. soln. KI gave I.MeI, m. 209° (decompn.) (H2O). 4-Acetyl-3-amino-2-phenylquinoline (1 g.) refluxed 1 h. with 10 cc. HCONH2 and 7 cc. AcOH gave 4-methyl-10-phenyl-1,3,9-triazaphenanthrene, needles, m. 157° (EtOAc or ligroine). I (2.5 g.) heated 0.75 h. with 10 cc. H2O2 in 20 cc. AcOH gave VIII (AcOH-HCONMe2). The AcOH mother liquors and residues heated 2 h. at 75-80° with 200 cc. H2O2 gave a compd. (XII), m. 330° (decompn.). XII was identical with the product obtained from VIII under the above conditions. IV (1 g.) heated 0.5 h. at 160° with 4 g. CO(NH2)2 then warmed with 20 cc. H2O, acidified with 1 cc. concd. HCl, and the filtrate basified gave VI. VIII (1 g.) in 10 cc. 3N NaOH shaken 15 min. at 60-70° with 1 cc. Me2SO4 gave 1(or 3)-methyl-4-oxo-10-phenyl-1,3,9-triazaphenanthrene, needles, m. 174-5° (alc.). IX (0.6 g.) and NaOMe refluxed 20 min. gave 4-methoxy-10-phenyl-1,3,9-triazaphenanthrene, needles, m. 163° (ligroine). They were inactive against Streptococcus (hemolytic), Staphylococcus aureus, Escherichia coli, Candida albicans, Plasmodium berghei, B. rodhaini, Trypanosoma equiperdum, T. congolense, and T. cruzi.

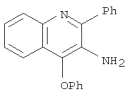
IT 102241-29-2
(Derived from data in the 6th Collective Formula Index (1957-1961))

RN 102241-29-2 CAPLUS

CN Quinoline, 3-amino-4-phenoxy-2-phenyl- (6CI) (CA INDEX NAME)

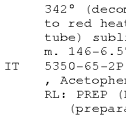


L4 ANSWER 22 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:25579 CAPLUS
DOCUMENT NUMBER: 52:25579
ORIGINAL REFERENCE NO.: 52:4657d-g
TITLE: Syntheses of kinetin analogs. I
AUTHOR(S): Okumura, F. Shigeo; Masumura, Mitsuo; Motoki, Toshiyuki; Takahashi, Tadashi; Kuraishi, Susumu
CORPORATE SOURCE: Tokushima Univ., Tokushima, Japan
SOURCE: Bulletin of the Chemical Society of Japan (1957), 30, 194-5
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB 6-Substituted purines (I) and 6-substituted 3-methylpyridazines (II) are prepared by condensing 6-methylthiopurine and 6-chloro-3-methylpyridazine, resp., with various amines. Typical I prepared by this method were [6-substituent, reaction temperature and time (hrs.), % yield, m.p. given]: 2-thenylamino (III), 120-30°, 12 (under H), 19.3, 247-7.5° (absolute alc.); III, 120-5°, 10 (sealed tube), 39.9, -; PhCH2NH (IV), 120-5°, 10 (sealed tube), 44.3, 229-30° (absolute alc.); MeCHPhNH (V), 120-30, 8 (under H), 54.2, 240-1° (absolute alc.); AmNH, 90-100°, 15 (under H), 36.7, 164-5° (C6H6); n-C6H13NH (VI), 130-5°, 9, 31.0, 177-8° (60% alc.); p-MeOC6H4CH2NH, 120-30°, 8 (under H), 48.2, 233-4° (absolute alc.); 3,4-(MeO)2C6H3NH, 120-5°, 10 (sealed tube), 48.1, 240.5-1.0° (absolute alc.); 3,4-CH2O2C6H3CH2NH, 120-30°, 12 (under CO2-free air), 40.3, 259-60° (absolute alc.); furfurylthio (prepared from 6-mercaptopurine and furfuryl chloride), -, -, 26.2, 174-5° (60% alc.). Typical II prepared (all in sealed tubes) were (6-substituent shown): 2-furfurylamino, 125°, 24, 66.0, 161-2° (C6H6); PhCH2NH, 100-30°, 18, 59.0, 138.5-9.0° (C6H6); PhNH, 100°, 1, 56.0, 167.5-8.0° (H2O); p-MeOC6H4CH2NH, 125°, 18, 79.5, 142-3° (C6H6); 2-thenylamino, 130°, 20, 81.0, 178-9° (alc.); 3,4-(MeO)2C6H3CH2NH, 135-40°, 16, 49.6, 127-8° (H2O). III, IV, and VI have the same effect on the growth of Raphanus leaf as does kinetin but V shows no activity (no verifying data given).
IT 102241-29-2
(Derived from data in the 6th Collective Formula Index (1957-1961))
RN 102241-29-2 CAPLUS
CN Quinoline, 3-amino-4-phenoxy-2-phenyl- (6CI) (CA INDEX NAME)

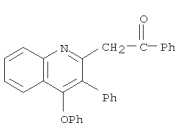


L4 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1956:24187 CAPLUS
DOCUMENT NUMBER: 50:24187
ORIGINAL REFERENCE NO.: 50:4954g-i,4955a-e
TITLE: A new method for the synthesis of certain benz[a]acridines
AUTHOR(S): Hauser, Charles R.; Murray, James G.
CORPORATE SOURCE: Duke Univ., Durham, NC
SOURCE: Journal of the American Chemical Society (1955), 77, 3858-60
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 50:24187
AB Certain 5-substituted benz[a]acridines were synthesized by acylating the Me group of 3-phenylquinaldine (I) or a derivative with an ester, and cyclizing the resulting ketone with polyphosphoric acid (II). PhCH2Ac (0.15 mol) and isatin were converted in the presence of alkali by the method of Borsche and Vorbach (C.A. 33, 1734.3) to 2-methyl-3-phenylcinchoninic acid, m. 338° (decomposition); the acid (50 g.) and 17 g. Cu powder, heated 2 h. at 340-50°, the mixture cooled, stirred with C6H6, and filtered, the solvent evaporated, and the residue distilled gave 35.4 g. I, yellow oil, b1.7 164°. I and (CO2Et)2 treated in the presence of KOEt by the method of Borsche and Vorbach (loc. cit.) gave Et (3-phenyl-2-quinolyl)pyruvate (III), orange needles, m. 161-3° (decomposition) (from EtOH). II (1.0 g.) and 10 g. II heated 15 min. at 195°, cooled to 85°, stirred with 20 cc. H2O, and filtered, the solid filter residue suspended in H2O, the mixture neutralized with 20% aqueous NaOH and filtered, and the residue triturated with hot 95% EtOH gave 0.67 g. benz[a]acridine-5-carboxylic acid (IV), yellow powder, m. 340° (decomposition); a 200-mg. portion sublimed gave 0.165 g. pure IV, m. 348° (decomposition). IV (0.100 g.) heated 0.5 h. with 0.1 g. Cu powder at 340° and the mixture sublimed at 140° and 0.5 mm. gave 0.047 g. benz[a]acridine (V), yellow needles, m. 132-3°. III (16.4 g.) in Et2O added to NaNH2 from 3.45 g. Na in liquid NH3, the mixture stirred 10 min., treated with 9.6 g. BzOMe in Et2O, stirred 4 h. at room temperature to evaporate the NH3, refluxed 0.5 h., diluted with H2O, and filtered, the Et2O layer of the filtrate evaporated to give addnl. solid, and the combined solids recrystd. from EtOH gave 12.0 g. 2-BzCH2 derivative (VI) of I, bright orange needles, m. 169-70° (from EtOH). VI (1 g.) heated 1.5 h. with 20 g. II at 195°, the mixture decomposed with H2O, neutralized with 20% aqueous NaOH, and extracted with Et2O, the extract washed, dried, and evaporated, and the residue recrystd. from 95% EtOH and dried on the steam bath yielded 0.82 g. 5-Ph derivative of V, yellow needles, m. 146-7° (sublimed at 160°/0.44 mm., recrystd. from 95% EtOH, and dried at 100°); picrate, yellow needles, m. 289-90° (from EtOH)

L4 ANSWER 23 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
(decompn.). 4-Cl deriv. of I (20 g.), 9.3 g. PhONa, and 40 g. PhOH refluxed 4 h., the mixt. basified strongly with 20% aq. NaOH and extd. with Et2O, the ext. evapd., and the residue washed with 20% aq. NaOH and H2O and recrystd. from 95% EtOH gave 19.8 g. 4-PhO deriv. (VII) of I, colorless crystals, m. 123-6° (from 95% EtOH). VII (9.36 g.) in Et2O added to NaNH2 from 1.38 g. Na in liq. NH3, the mixt. stirred 5 min., treated with 8.16 g. BzOMe in Et2O, and stirred 1.5 h., the NH3 evapd., the residual Et2O suspension refluxed 8 h., dild. with H2O, and filtered, and the solid recrystd. from EtOH yielded 6.4 g. 4-PhO deriv. (VIII) of VI, orange plates, m. 185.5-87° (from EtOH). VIII (3 g.) heated 2.5 h. at 195° with 30 g. II, the mixt. decompd. with H2O and filtered, the residue suspended in 120 cc. N NaOH and extd. with Et2O, the ext. evapd., and the residue recrystd. from 95% EtOH yielded 1.60 g. 5-phenyl-12-phenoxy deriv. (IX) of V, light yellow crystals, m. 207-9°. IX hydrolyzed with HBr gave 12(7H)-oxo deriv. (X) of 5-phenylbenz[a]acridine (XI). The crude solid (1.0 g.) from VIII and II refluxed with 5 cc. 48% HBr, 20 cc. EtOH, and 5 cc. H2O 3 h. with stirring, the mixt. neutralized with NaOH and filtered, and the solid washed with H2O and Et2O and triturated with hot EtOH gave 0.39 g. X, m. 342° (decompn.) (sublimed). X (0.25 g.) heated with 20 g. Zn dust to red heat and the distillate (collected on the wall of the combustion tube) sublimed at 160° and 0.4 mm. and recrystd. from EtOH gave XI, m. 146-6.5°.
IT 5350-65-2P, Quinaldine, 4-phenoxy-3-phenyl- 652972-11-7P , Acetophenone, 2-(4-phenoxy-3-phenyl-2-quinolyl)-
RL: PREP (Preparation)
(preparation of)
RN 5350-65-2 CAPLUS
CN Quinoline, 2-methyl-4-phenoxy-3-phenyl- (CA INDEX NAME)

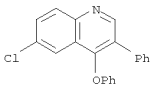


RN 652972-11-7 CAPLUS
CN Acetophenone, 2-(4-phenoxy-3-phenyl-2-quinolyl)- (5CI) (CA INDEX NAME)



L4 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1951:36166 CAPLUS
DOCUMENT NUMBER: 45:36166
ORIGINAL REFERENCE NO.: 45:6204f-i,6205a-b
TITLE: Some 4-(dialkylaminoalkylamino)-3-phenylquinolines
AUTHOR(S): Adams, W. J.; Hey, D. H.
CORPORATE SOURCE: Univ. London
SOURCE: Journal of the Chemical Society (1950) 3254-9
CODEN: JCSOA9; ISSN: 0368-1769
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB The amine (1 mol.) is added to 1 mol. HCOCHPhCO2Et (I) at room temperature (slight warming in the case of solid amines), kept 24 hrs. at room temperature, the product extracted with ether, and the oil added to boiling Ph2O and heated for varying times, giving 21-55% of the following 4-hydroxy-3-phenylquinolines (II): 6-Cl, m. 349-9.5° (decomposition); 8-Cl, cream, m. 248-51°; 6-Br, cream, m. 365° (decomposition); 6-NO2, yellow, m. 349-50° (decomposition); 8-NO2, bright orange, m. 215-16°; 6-MeO, m. 337-8° (decomposition). The II (1 mol.) and 1 mol. PCl5 in POCl3 were heated from 25 min. to 1.5 hrs., giving the 4-chloro-3-phenylquinolines (III): 6-Cl, m. 144.5°; 8-Cl, m. 112.5-13.5°; 6-NO2, pale brown, m. 170.5-2°; 6-MeO, yellow, m. 138-8.5° (picrate, yellow, m. 206-7°); in 1 experiment the product was 4,x-dichloro-6-methoxy-3-phenylquinoline, m. 131-1.5°. 4-Chloro-3-phenylquinoline (0.5 g.) and 0.2 g. PhNH2, heated 5 min. at 130° and the product extracted with 5% HCl, give the HCl salt, bright yellow, m. 300°, of 4-anilino-3-phenylquinoline (IV), cream, m. 179.5-80.5°; 6-MeO derivative, cream, m. 172-3°. The III (1 mol.) and 2.5 mols. of the amine were heated 4 hrs. at 160-80° and 4 hrs. at 210°, the excess amine removed in vacuo, the residue extracted with 66% aqueous AcOH, the solution made alkaline with 10% aqueous NaOH, the oil extracted with ether, diluted with AcOH, and the base precipitated with picric acid, giving the dipicrates of 3-phenylquinolines (the Me2CO of crystallization is removed at 100° in vacuo but not at 80° at atmospheric pressure): 4-(2-diethylaminoethylamino), m. 201.5-2.5° (all m. with decomposition) (6-Cl derivative, with 1 mol. Me2CO, m. 202.5-4.5°; 7-Cl derivative, with 1 mol. Me2CO, m. 205-6°; 6-MeO derivative, with 1 mol. Me2CO, m. 170-3°); 4-(4-diethylamino-1-methylbutylamino), m. 213-15°; 6-Cl derivative with 1 mol. Me2CO, m. 210-18°; 7-Cl derivative, with 1 mol. Me2CO, m. 205-6°; 6-MeO derivative, with 1 mol. Me2CO, m. 194-5°. 6-Chloro-4-phenoxy-3-phenylquinoline, m. 152.5-3.5°. α-Phenyl-p-acetanisidide m. 122-3° (from PhCH2COCl and p-MeOC6H4NH2). Impure I and amines give α-phenylacetanilides. PhNH2 (1.9 g.) and 3.8 g. I, 24 hrs. at room temperature, give 48% 4-hydroxy-3-phenylquinoline (V), and 0.7 g. IV; the reactants, 30 min. at room temperature and 24 hrs. at room temperature, give 45% V and 0.5 g. IV; heating 30 min. at 100° and keeping 24 hrs. at room temperature gives 34% V and 0.2 g. IV; thus, temperature has little effect on the reaction. I and PhNH2 (0.02 mol. each) give 41% V; 0.02 mol. I and 0.018

L4 ANSWER 24 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)
mol. PhNH2 give 59% V; 0.02 mol. I and 0.04 mol. PhNH2 give 5% V, 22% IV, and 1.7 g. (PhNH)2CO. The PhNHCH:CPhCO2Et (from 3.8 g. I and 1.7 g. PhNH2), cyclized in 20 or 40 cc. Ph2O, gives 47 and 81% V, resp.
IT 860719-92-2P, Quinoline, 6-chloro-4-phenoxy-3-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 860719-92-2 CAPLUS
CN Quinoline, 6-chloro-4-phenoxy-3-phenyl- (CA INDEX NAME)



L4 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1928:20202 CAPLUS
DOCUMENT NUMBER: 22:20202
ORIGINAL REFERENCE NO.: 22:2358h-i
TITLE: Quinoline derivatives. VIII. Compounds of 2-phenyl-4-hydroxyquinoline
AUTHOR(S): John, Hanns; Wunsche, E.
SOURCE: Journal fuer Praktische Chemie (Leipzig) (1928), 119, 43-8
CODEN: JPCEAO; ISSN: 0021-8383
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C. A. 22, 426. 2-Phenyl-4-acetoxyquinoline, m. 70°; picrate. BzO derivative, m. 90-1°; picrate, 4-EtO derivative, m. 100 2°; various salts of this and the following are described. 4-PhO derivative, pale
yellow, m. 252°. 4-m-Cresoxy derivative, m. 241-3°. 4-p-Nitrophenoxy derivative, m. 88-90°. 4-p-Aminophenoxy derivative, m. 81°. 4-o-Methoxyphenoxy derivative, m. 246°. 4-o-Isopropyl-m-methylphenoxy derivative, m. 252°. All but the 1st two derivs. were prepared from the 4-Cl derivative
IT 855837-34-2P, Quinoline, 4-(p-aminophenoxy)-2-phenyl- 856088-26-1P, Quinoline, 2-phenyl-4-m-toloxy- 856088-31-8P, Quinoline, 4-(p-nitrophenoxy)-2-phenyl- 856096-43-0P, Quinoline, 4-(2-isopropyl-5-methylphenoxy)-2-phenyl- 856096-70-3P, Quinoline, 4-phenoxy-2-phenyl- 856096-92-9P, Quinoline, 4-(o-methoxyphenoxy)-2-phenyl-
RL: PREP (Preparation)
(preparation of)
RN 855837-34-2 CAPLUS
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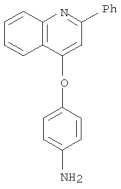
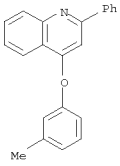


RN 856088-26-1 CAPLUS
CN Quinoline, 2-phenyl-4-m-toloxy- (3CI) (CA INDEX NAME)

L4 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



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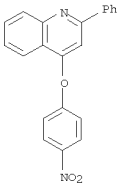

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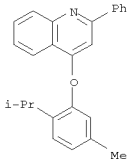

RN 856096-70-3 CAPLUS
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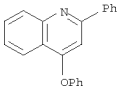
L4 ANSWER 25 OF 25 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



RN 856096-92-9 CAPLUS
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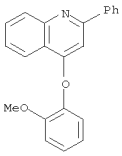

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